Next Generation Nuclear Plant

TRISO-coated Fuel Performance Modeling: The PARFUME Code

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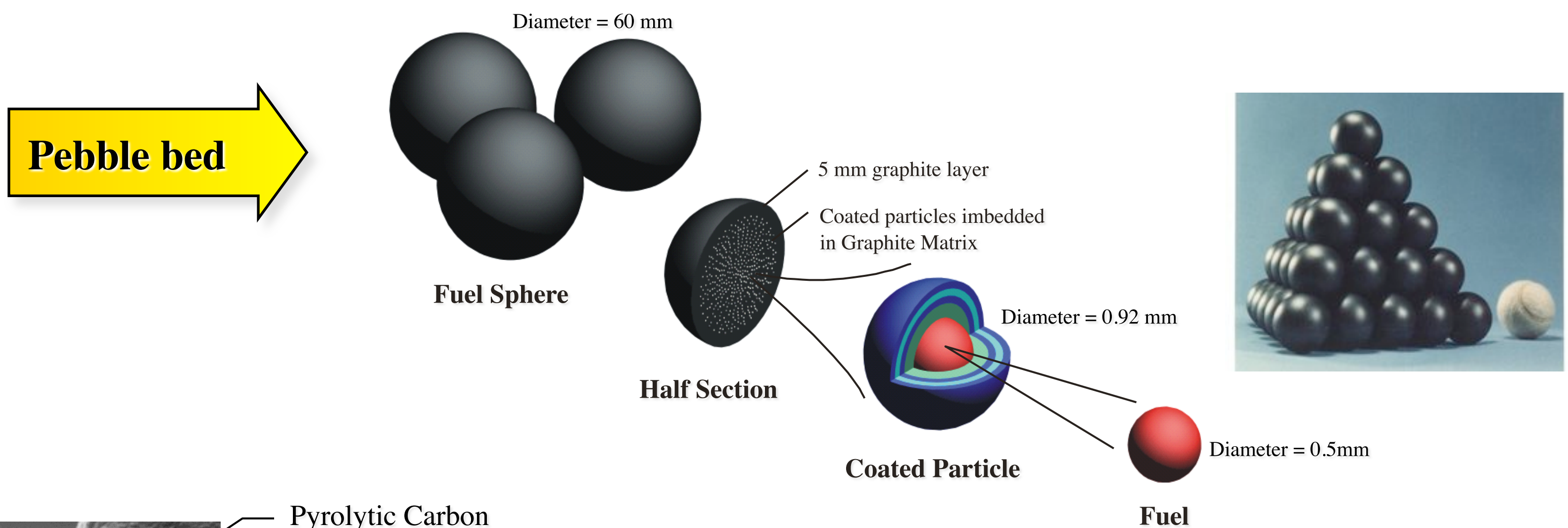
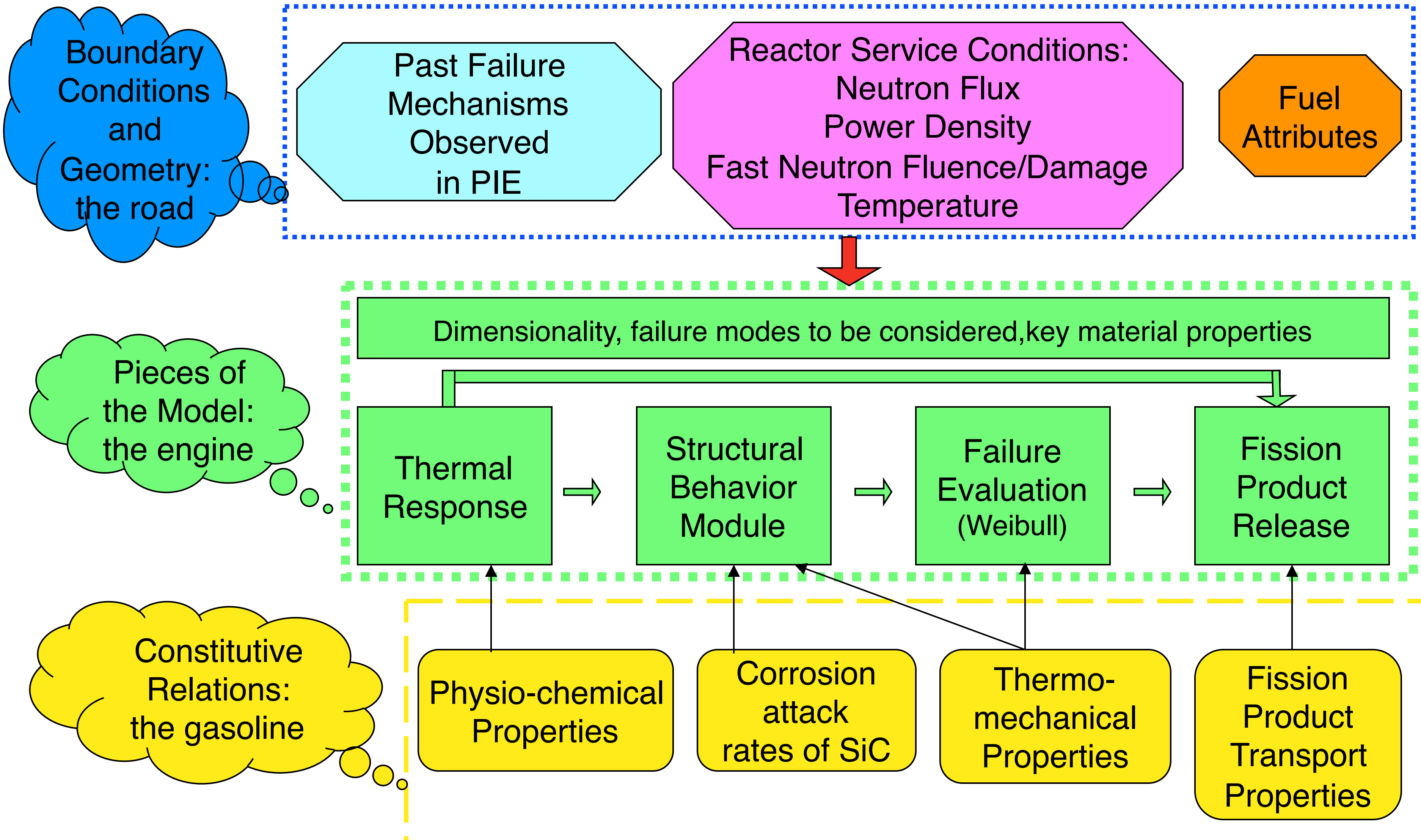
Background

All HTGRs Rely on Coated Particle Fuel



TRISO coating primary barrier for fission product release

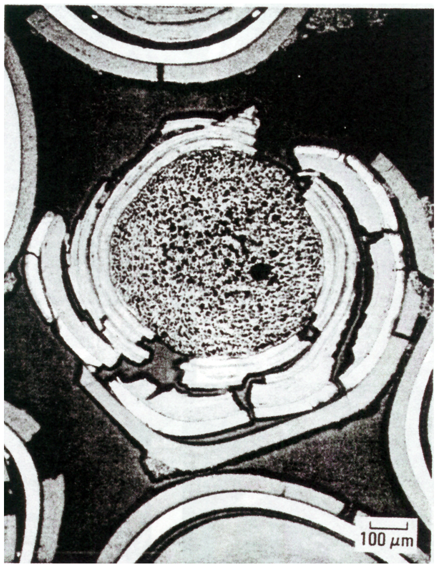
Overview of Approach for Particle Fuel Performance Modeling

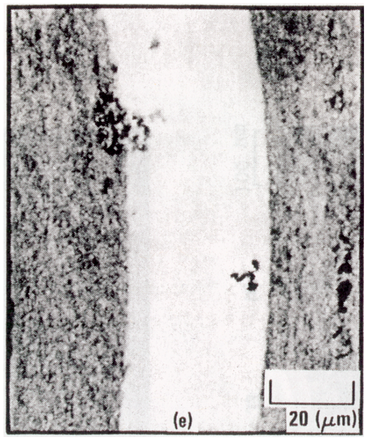


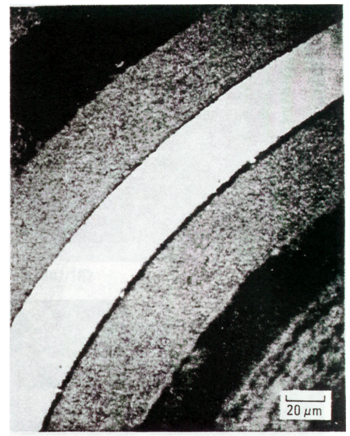
Overview of Approach for Particle Fuel Performance Modeling

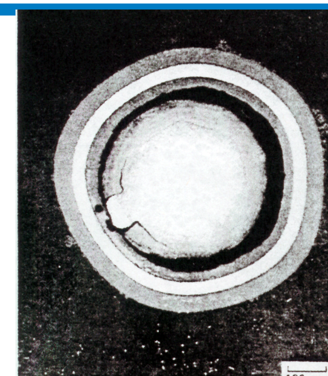
Past Failure
Mechanisms
Observed
in PIE

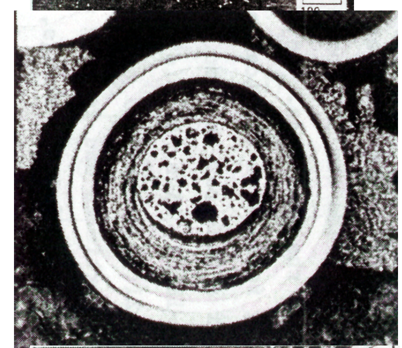
Inferred fuel failure mechanisms from US irradiations: Overpressure, IPyC Cracking, Ameoba Effect, FP Attack

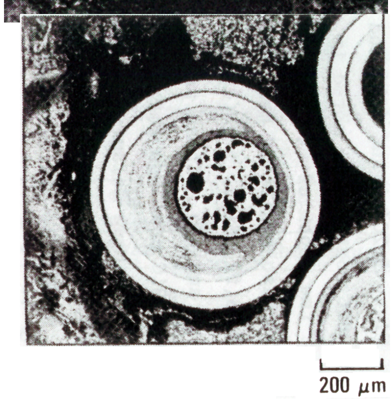


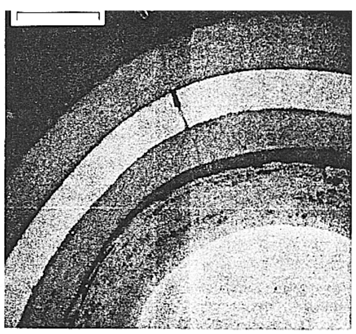


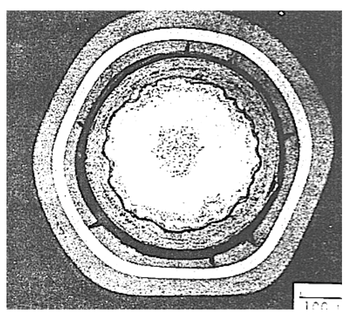


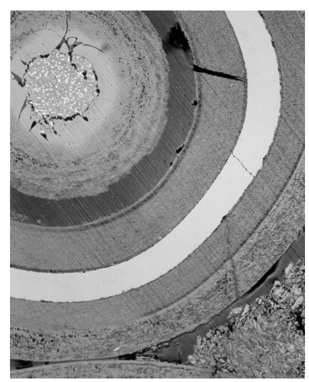








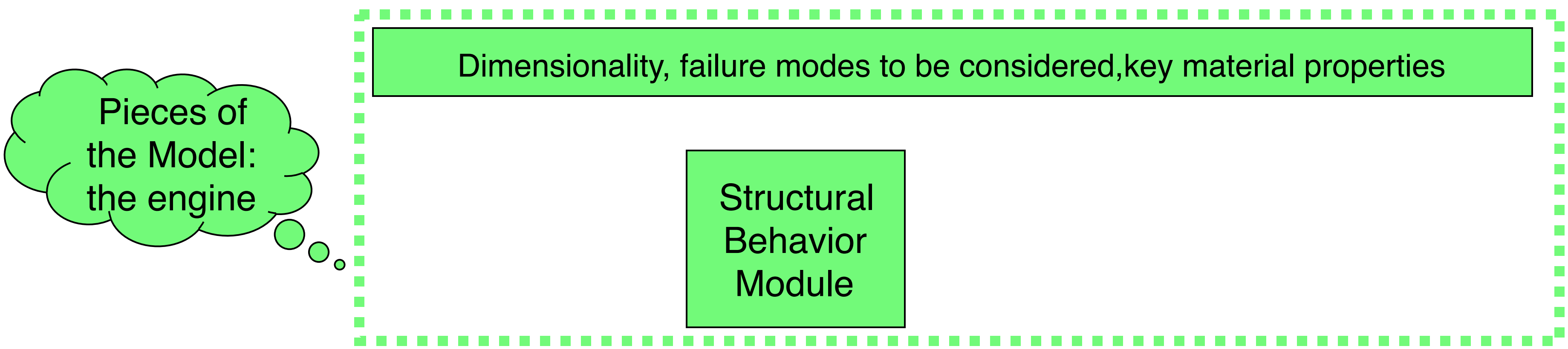




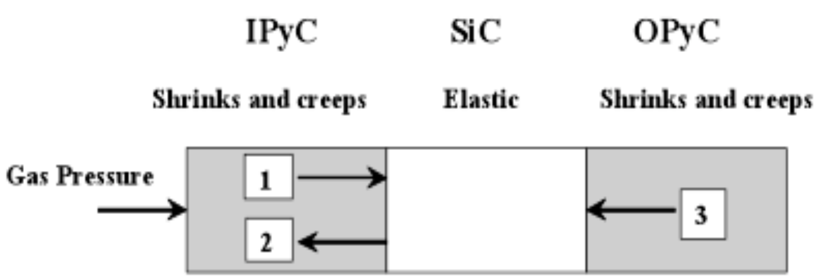
PARFUME Capabilities

Structural	Service Conditions	Physio-chemical	Layer Interactions	Failure
Intact particles	Any user specified temperature, burnup and fluence history	Booth equivalent sphere for fission gas release using Turnbull diffusivities	Amoeba effect	Mont Carlo based Sample
Cracked layers	Improved Thermal model for fuel element and particle	HSC thermodynamic based for CO production for any fuel composition	Fission product-SiC interactions (e.g. Pd)	Direct numerical integration
Debonded layers		Redlich-Kwong EOS	Thermal Decomposition	
Faceted particles		Fission product transport across each layer		

Overview of Approach for Particle Fuel Performance Modeling



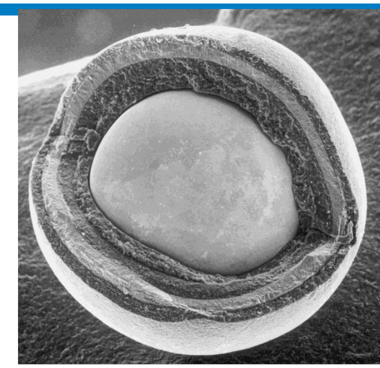
Behavior of Coating Layers in Standard Fuel Particle



1 Gas pressure is transmitted through the IPyC

2 IPyC shrinks, pulling away from the SiC

3 OPyC shrinks, pushing in on SiC



$$\varepsilon_r = \frac{\partial u}{\partial r}$$

$$\frac{\partial \varepsilon_r}{\partial t} = \frac{1}{E}\left(\frac{\partial \sigma_r}{\partial t} - 2\mu\frac{\partial \sigma_t}{\partial t}\right) + c(\sigma_r - 2\nu\sigma_t) + S_r + \alpha_r\dot{T}$$

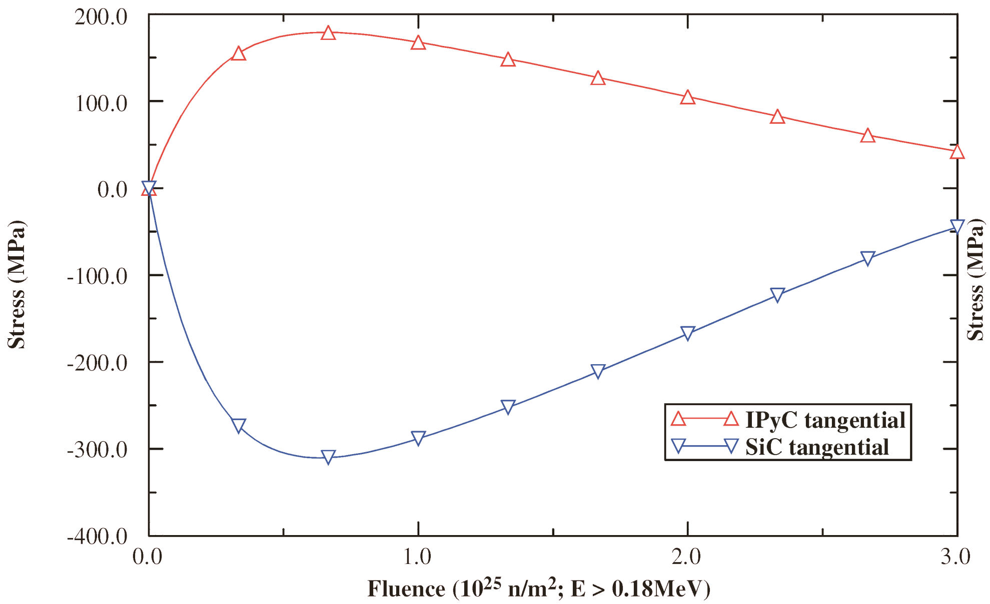
$$\varepsilon_t = \frac{u}{r}$$

$$\frac{\partial \varepsilon_t}{\partial t} = \frac{1}{E}\left((1-\mu)\frac{\partial \sigma_t}{\partial t} - \mu\frac{\partial \sigma_r}{\partial t}\right) + c[(1-\nu)\sigma_t - \nu\sigma_r] + S_t + \alpha_t\dot{T}$$

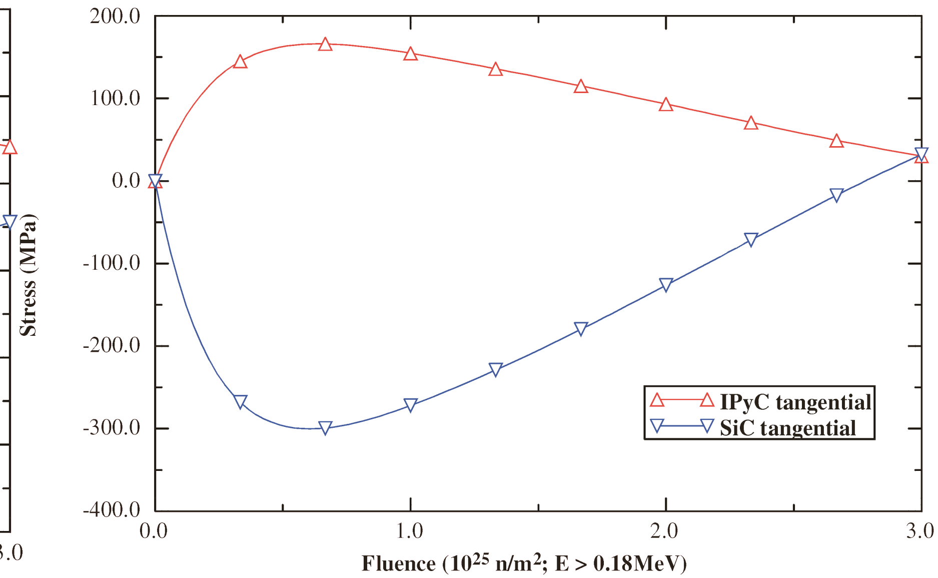
$$\frac{\partial \sigma_r}{\partial r} + \frac{2}{r}(\sigma_r - \sigma_t) = 0$$

Typical Stress Distribution in TRISO Coatings

350 μm kernel

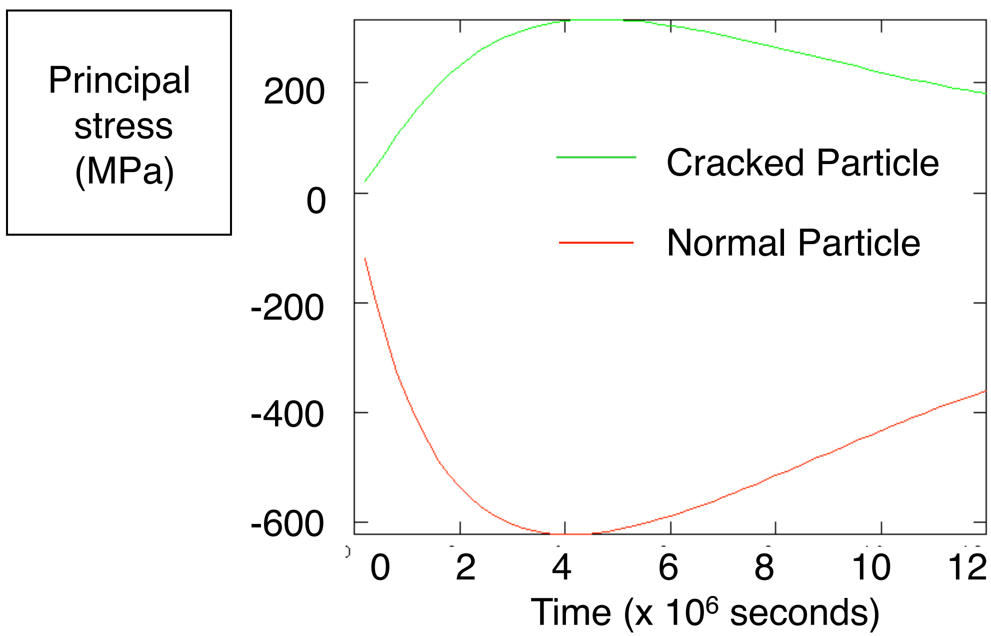


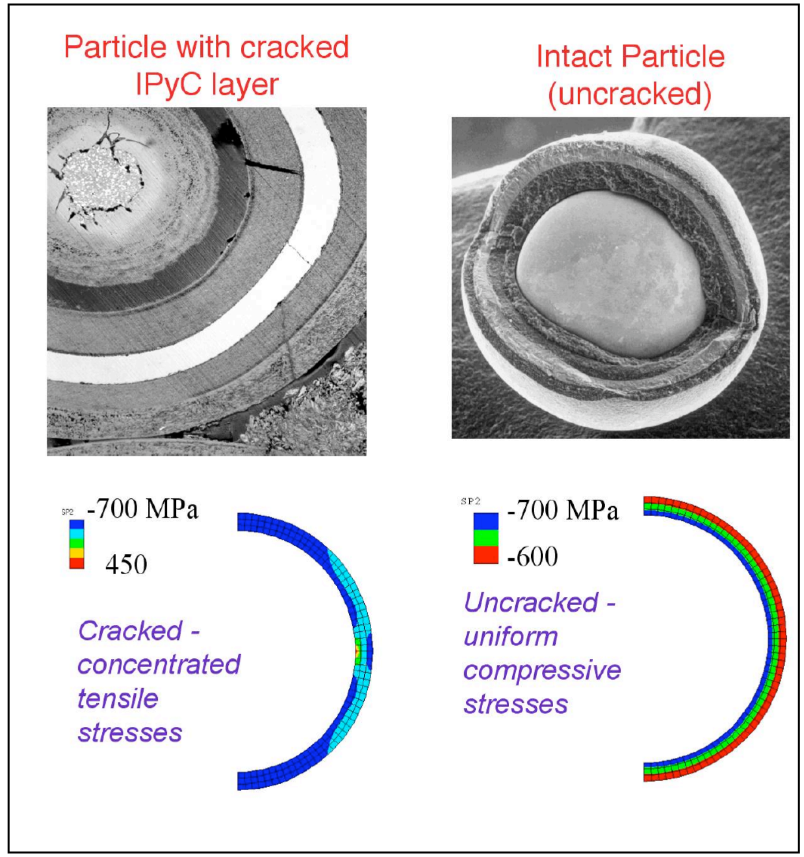
500 μm kernel



ABAQUS Results from Standard and Cracked Models

Standard/Nominal Particle is in compression; Particle with Cracked IPyC has SiC layer in tension

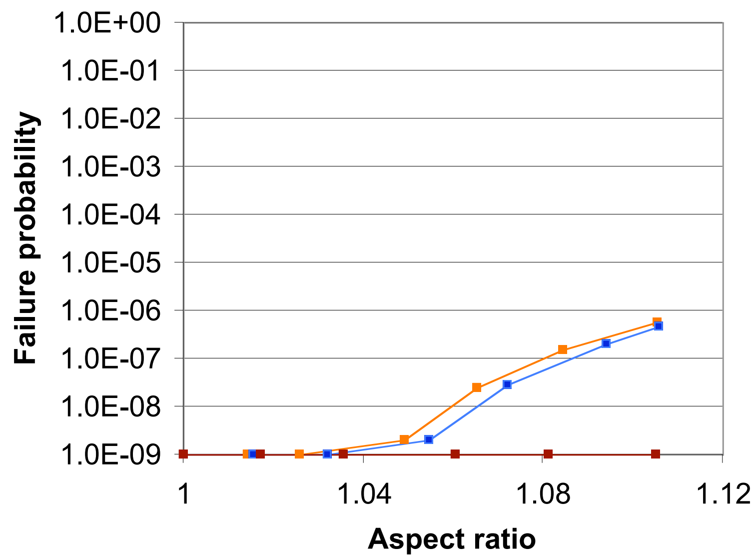


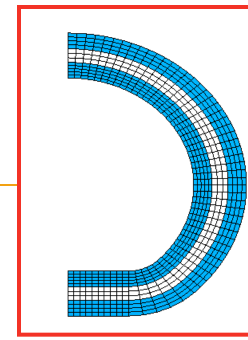


Note: Model contains ~ 800 nodes and takes about 2- 8 hours to run

PARFUME Calculations on Asphericity

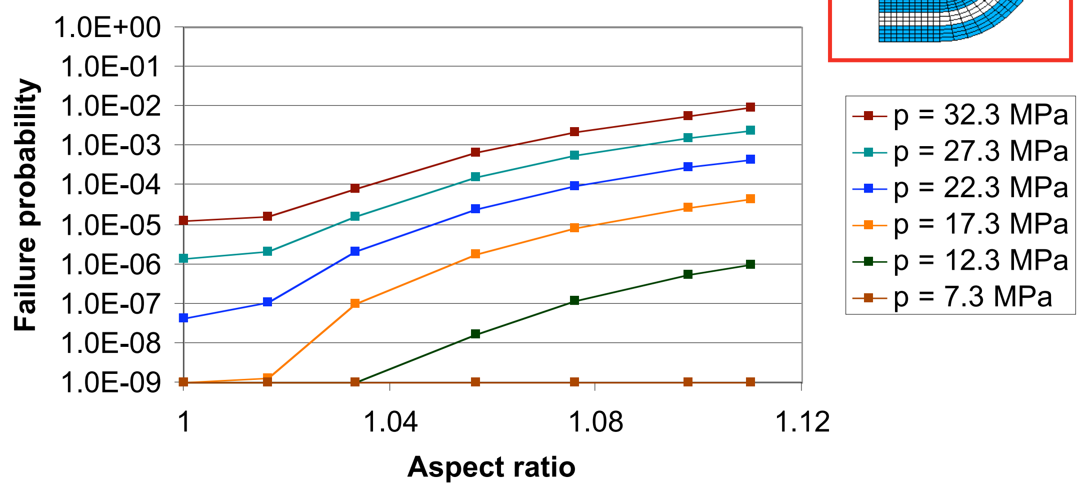
- Finite element based calculations of stress state
- Aspect ratio is a function of particle size
- Influence of pressure is very strong
- Could become important as coated particle fuel is pushed to high burnup or high temperature (accidents)

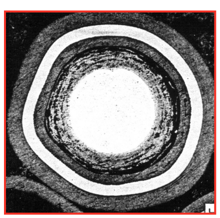


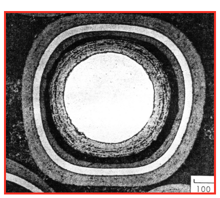


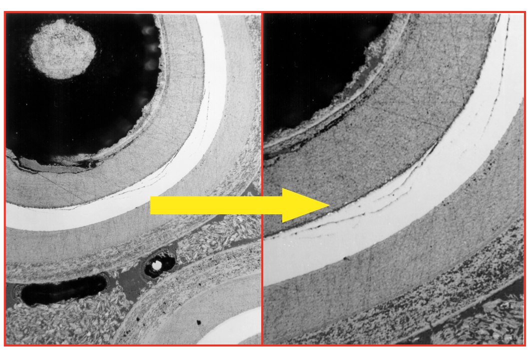
350 micron kernel

AGR



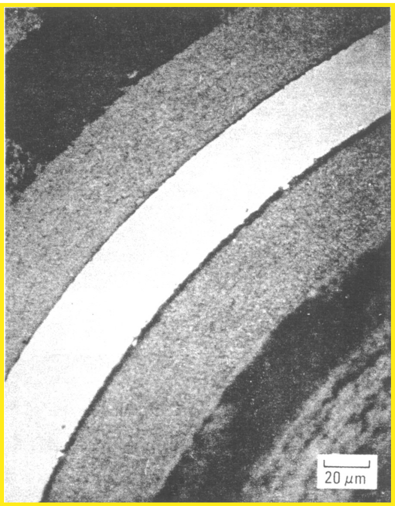


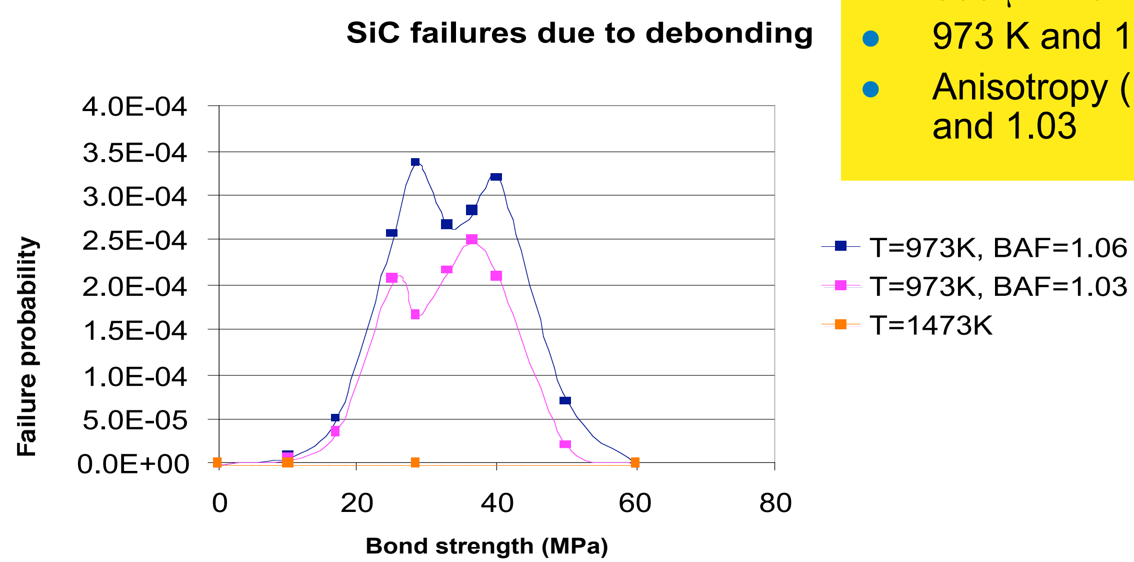


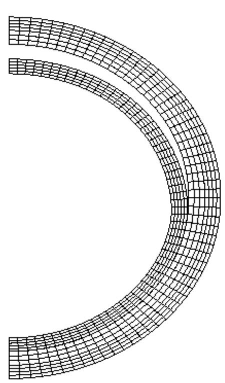


Debonding: Failure Probability as a Function of Bonding Strength

- 500 μm kernel
- 973 K and 1473 K
- Anisotropy (BAF) = 1.06 and 1.03

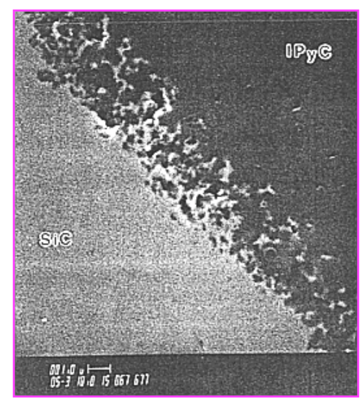






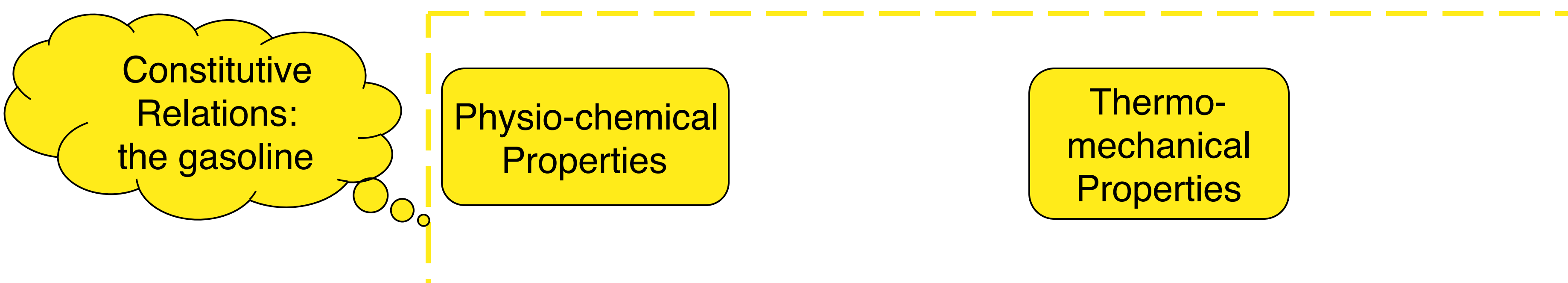
US - Weak

German and US interfacial bonding



German - Strong

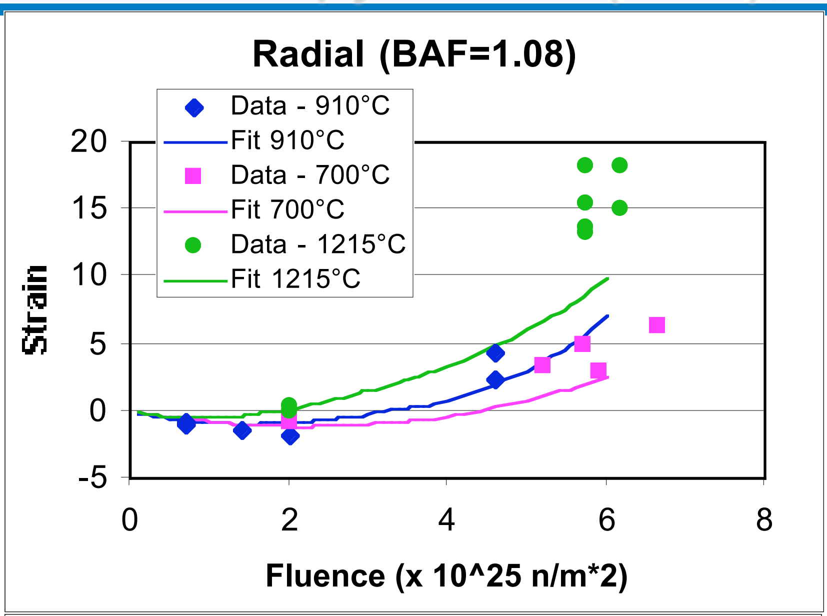
Overview of Approach for Particle Fuel Performance Modeling

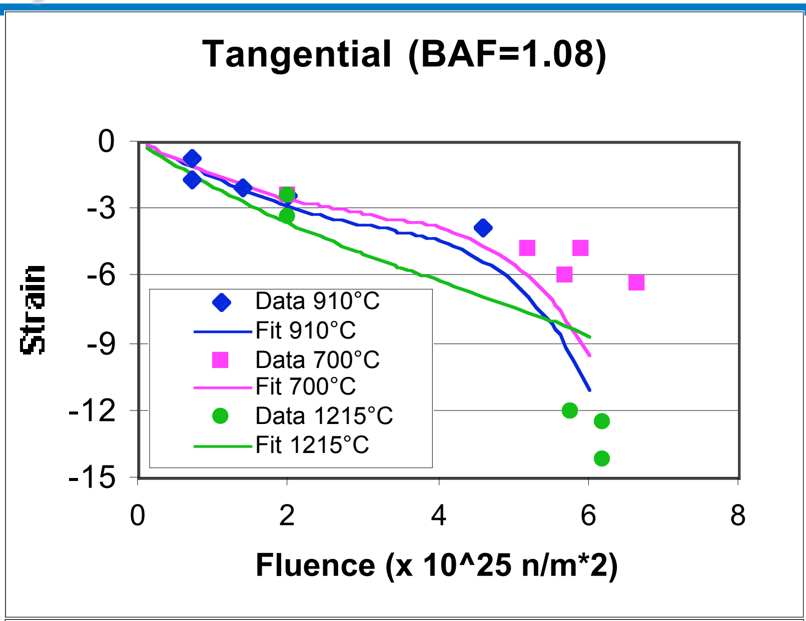


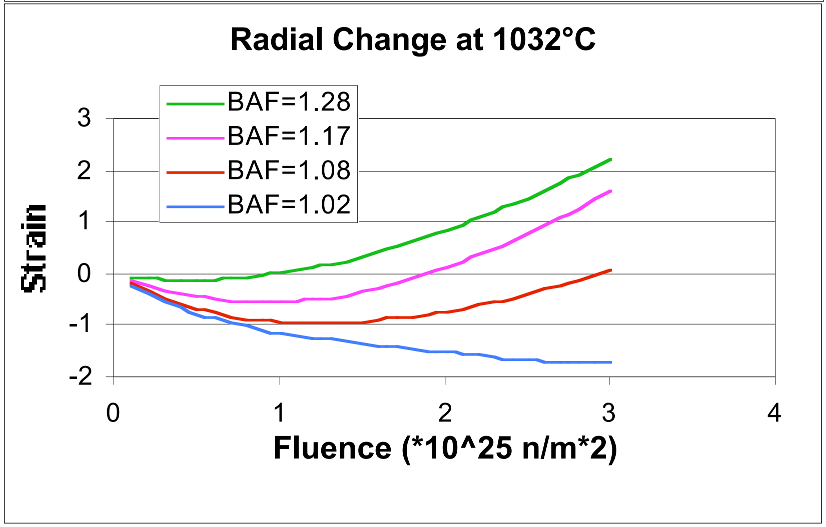
Key Materials Properties

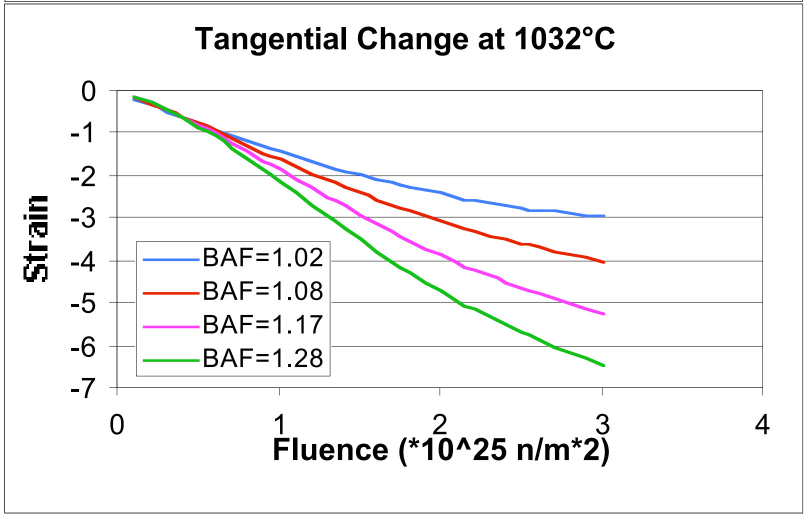
- Thermophysical and Thermomechanical
  - PyC Shrinkage/Swelling
  - PyC Irradiation Induced Creep
  - IPyC Change in Anisotropy under Irradiation
  - PyC CTE and Elastic Modulus
  - PyC Poisson's Ratio in Creep
  - PyC Fracture Strength/Failure Criteria
  - SiC Fracture Strength
- Physio-chemical
  - Fission Gas Release
  - Kernel Swelling
  - CO production (UO_2 fuel)
  - Pd interaction rate
  - Cs and Co interactions with SiC

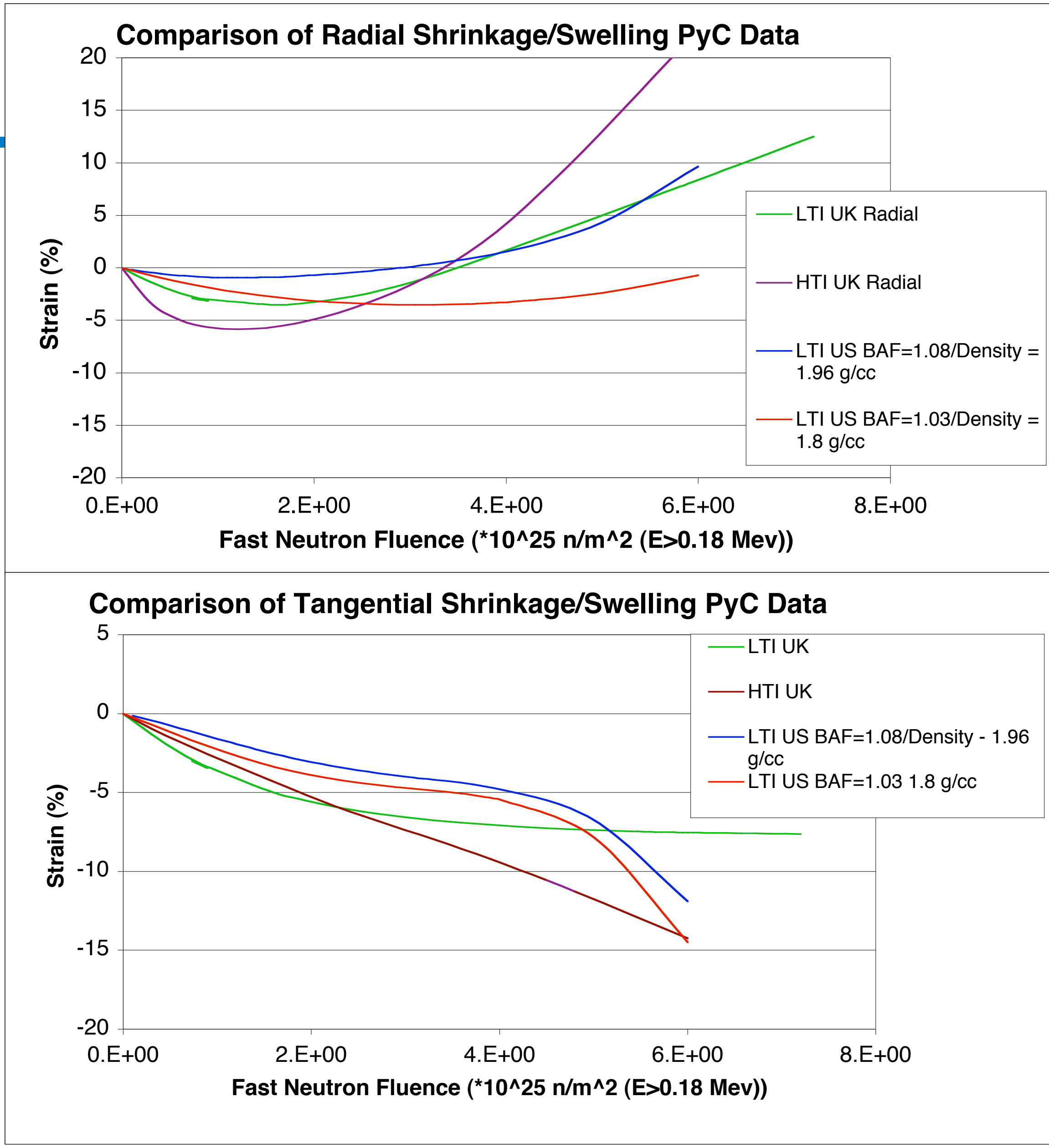
PyC shrinkage is a function of temperature, Bacon Anisotropy Factor (BAF), density and fluence







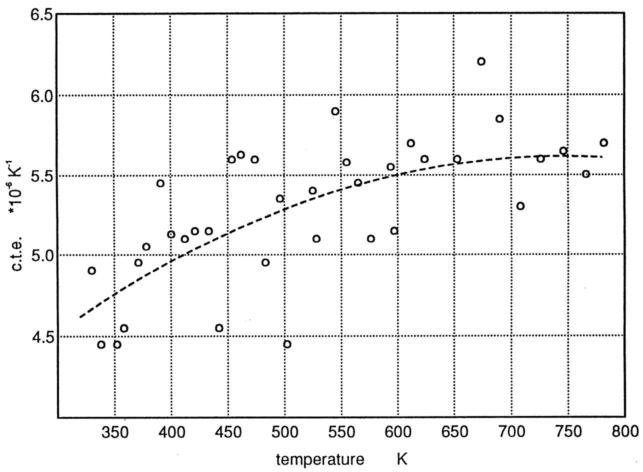




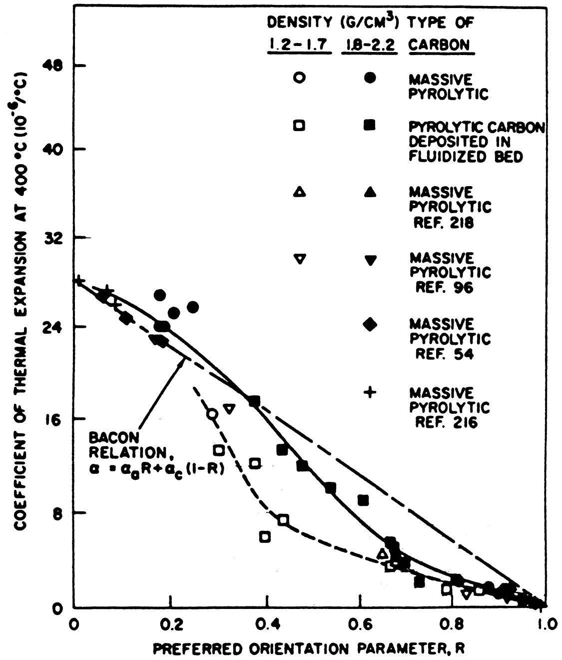
Comparison of GA and UK PyC Shrinkage Data:

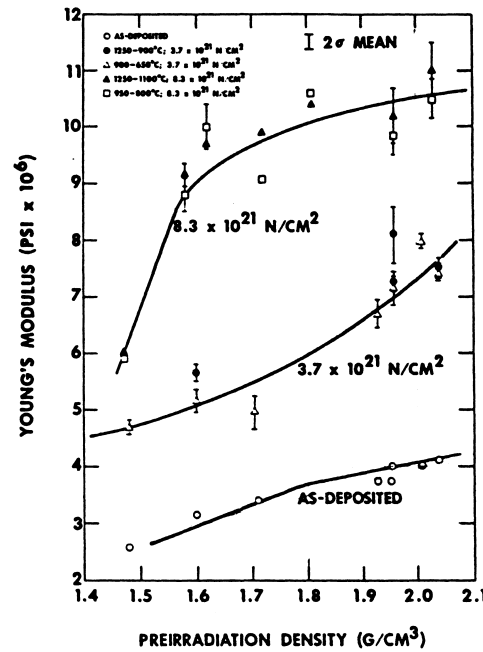
Similar shrinkage rates for similar conditions

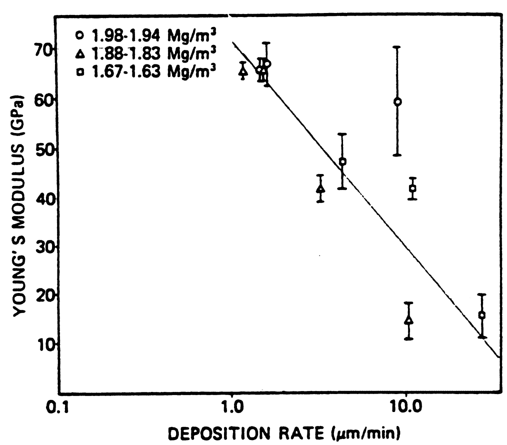
PyC CTE and Elastic Modulus are important to understand behavior in thermal transients in reactor and in experiments

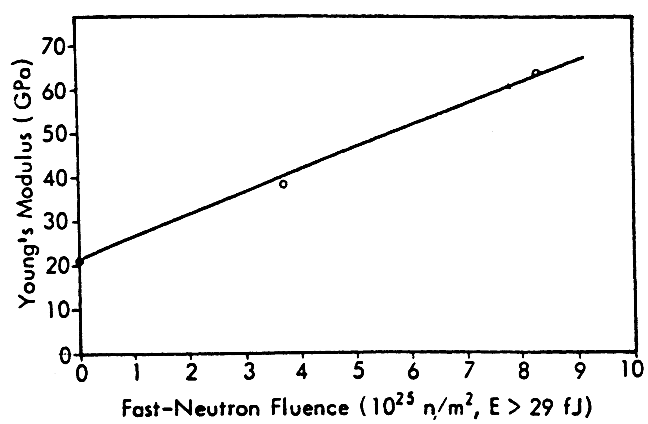


- CTE is different in the two orientations in PyC and depends on the anistropy of the material. Effect of irradiation is unknown
- Elastic modulus is a function of anisotropy, fluence, density and temperature



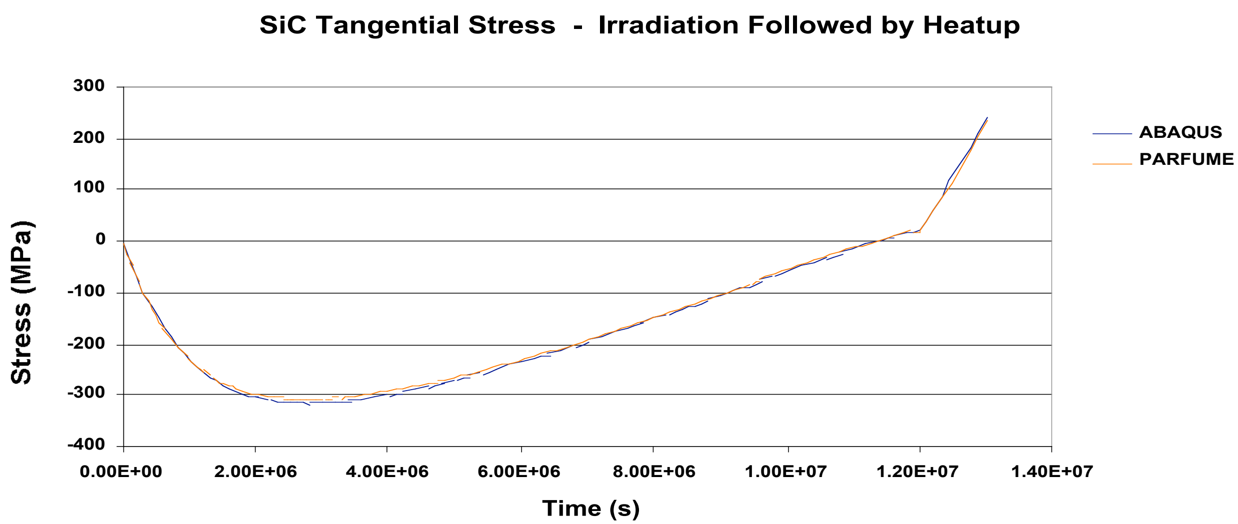






Comparison of ABAQUS and PARFUME accident simulation

- A sudden temperature increase due to an accident condition following a normal period of irradiation
  - Induces differential thermal expansion between layers and increases internal gas pressure
  - PARFUME solves for expansion concurrently with irradiation-induced creep and swelling, and internal pressure
- 500 μm particle; 70% FIMA; irradiated at 1273 K and then heated to 1673 K.



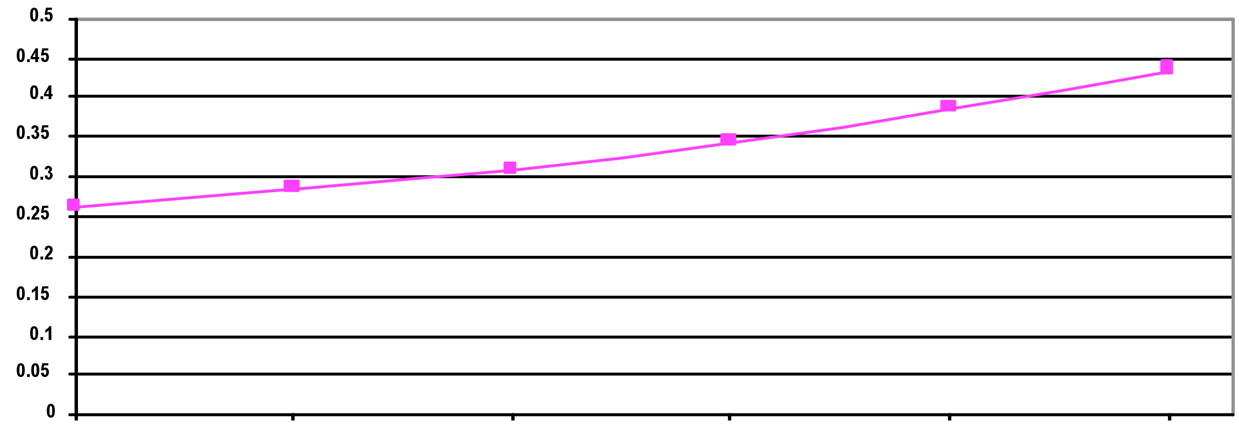
PARFUME Model Importance Assessment for Cracked Particle

Parameter	Nominal value	Range of variation	Influence factor
IPyC BAF	1.06	1.0 - 1.18	3.83
OPyC BAF	1.06	1.0 - 1.18	2.09
IPyC thickness (μm)	40	30 - 50	1.66
Creep 10^{-29}(MPa-n/m^2)$^{-1}$	2.71	1.36 - 4.75	1.55
SiC thickness (μm)	35	25 - 45	1.51
IPyC density (10^6 g/m^3)	1.9	1.8 - 2	1.20
Irradiation temperature (°C)	1000	600 - 1250	1.0
PoissonÕs ratio in creep	0.5	0.3 - 0.5	0.86
Kernel diameter (μm)	500	175 - 650	0.75
OPyC density (10^6 g/m^3)	1.9	1.8 - 2	0.71
OPyC thickness (μm)	40	30 - 50	0.55
Buffer thickness (μm)	100	80 - 120	0.19

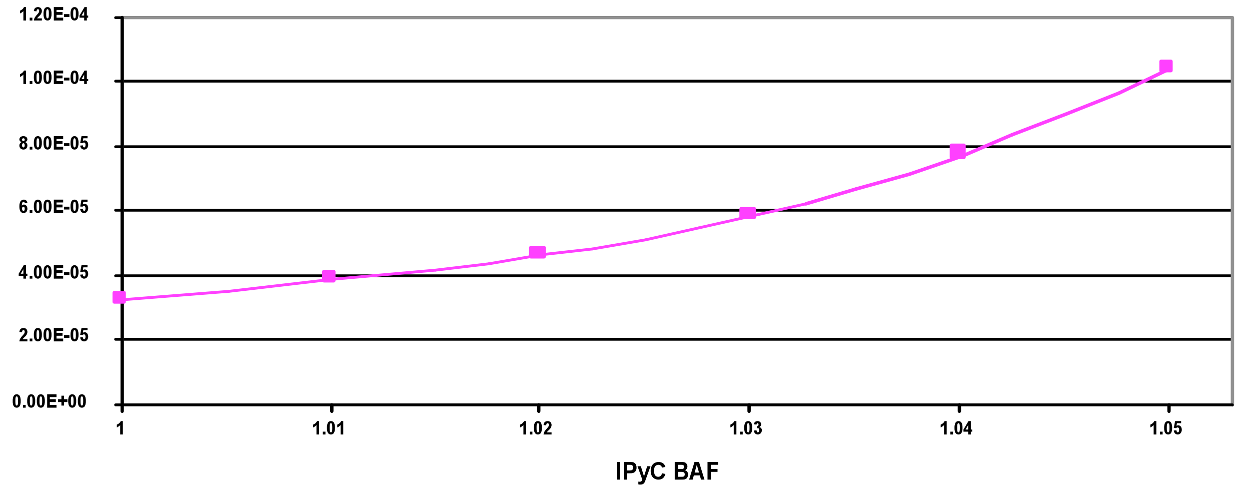
PyC Material properties are critical and highly uncertain!

IPyC Isotropy Calculation Results

IPyC failure probability vs. IPyC BAF

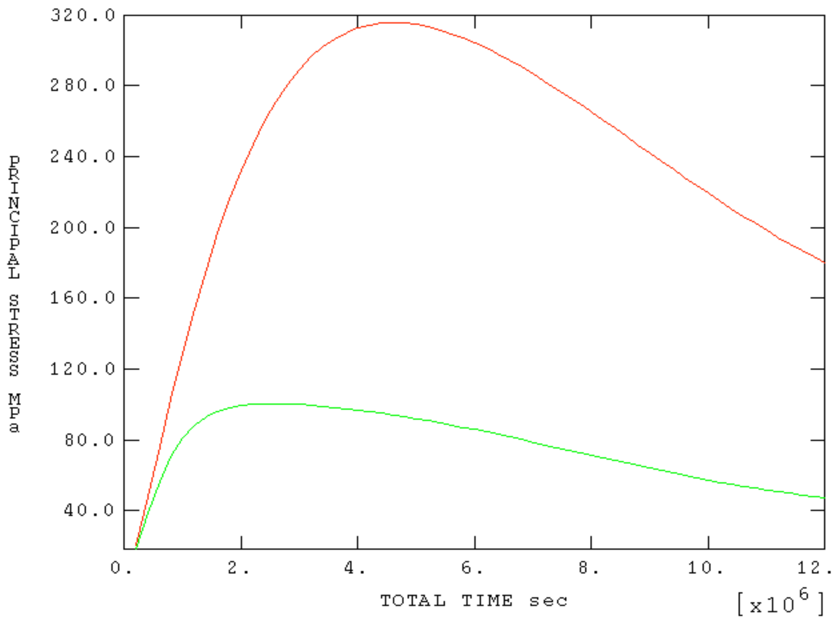


SiC failure probability vs. IPyC BAF



There is a wide range of PyC irradiation induced creep data in the literature and it has a large impact on calculated fuel performance

SiC Stress in Cracked Particle at 1200°C using different PyC creep data



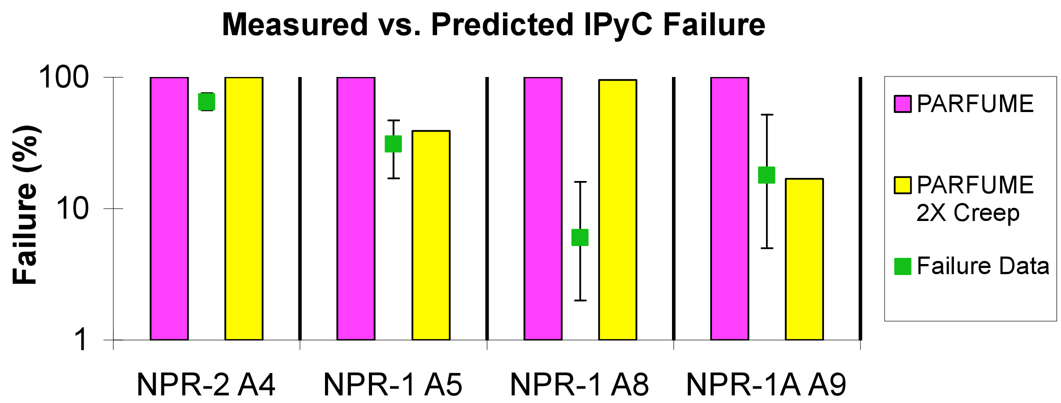
Using historical creep value of 4.29 $*10^{27}$ (psi-nvt)$^{-1}$ from GA

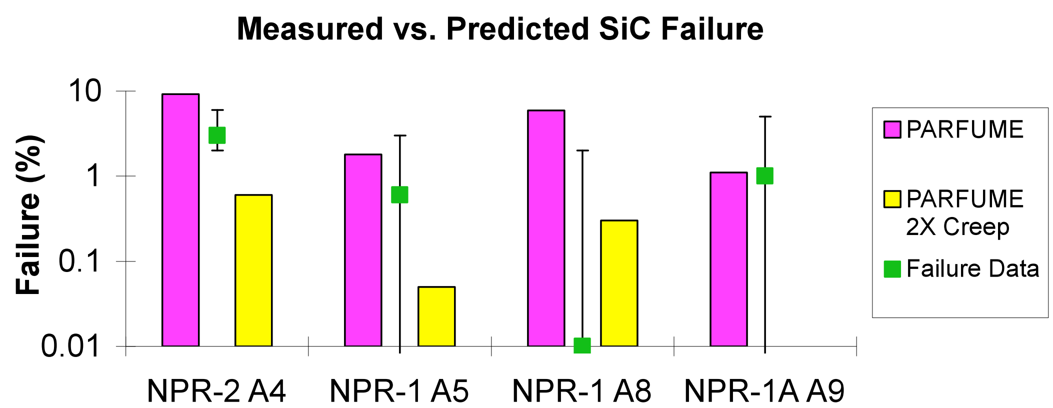
Using new creep value of 1.4$*10^{27}$ (psi-nvt)$^{-1}$ based on broad assessment of data from GA in 1993

Note: STRESS3 code uses 3.4 $*10^{27}$ (psi-nvt)$^{-1}$

Author	Creep constant (> 0.18 MeV) (x 10^{-29} MPa n/m^2)$^{-1}$
Kaae et al. (1972)	1.0
Price and Bokros (1967)	1.3
Buckley et al (1975)	4.8
Buckley et al. (1975)	4
Brocklehurst and Gilchrist (1976)	3.3 & 1.7
Morgand (1975)	13.2

PARFUME Predictions vs. Observations for NPR Experiments





Fuel Compact ID	Fast Fluence (10^{25} n/m^2)	Irradiation Temp. (°C)	Burnup (% FIMA)
NPR-2 A4	3.8	746	79
NPR-1 A5	3.8	987	79
NPR-1 A8	2.4	845	72
NPR-1A A9	1.9	1052	64

Effect of IPyC Poisson's ratio in creep on calculated stress in cracked particle

Case	IPyC Stress (MPa, tension)		SiC Stress (MPa, compression)	
	$\nu_c = 0.5$	$\nu_c = 0.4$	$\nu_c = 0.5$	$\nu_c = 0.4$
Nominal, T = 1273°K	475	351	847	697
Nominal, T = 873°K	627	488	1107	948
NPR-1 A9	430	307	784	610
NPR-2 A4	599	449	1101	895

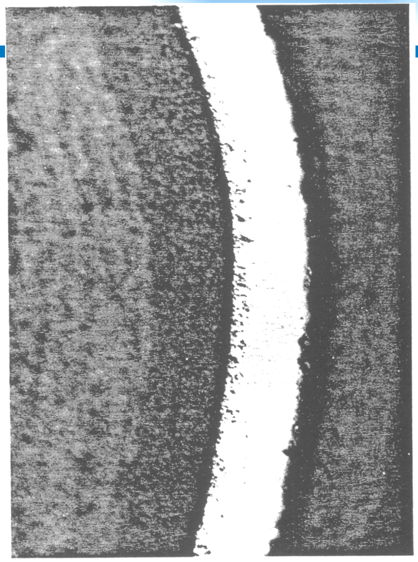
Note: range of values in literature is from 0.3 to 0.5

Key Material Property Measurements

- Key PyC and SiC properties are being measured for current generation of coated particles
  - PyC creep under accelerator (U-Michigan) and neutron irradiation (EU - PYCASSO irradiation)
  - SiC, ZrC, and PyC strength at ORNL. (Work on early generation of SiC already published)
  - Thermal conductivity of compacts during AGR PIEs (and by USU)
- Other key properties are under discussion in GIF VHTR fuels collaboration

High Burnup Issues

- German high temperature heating results suggest enhanced release from coated particles at burnups in excess of 12% FIMA and fluences in excess of 4×10^{25} n/m^2
- This behavior could be life limiting as HTGRs push to higher burnup
- Photomicrographs suggest a degradation of the SiC layer after long heating times
- Reason for the degradation is not clear
- We are studying two alternate hypotheses:
  - Cesium attack/interaction with SiC
  - CO reaction with the SiC



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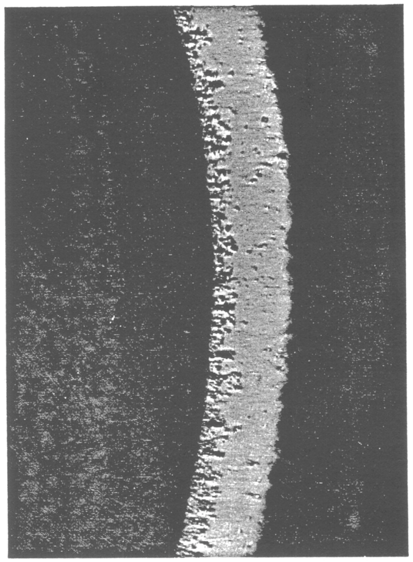
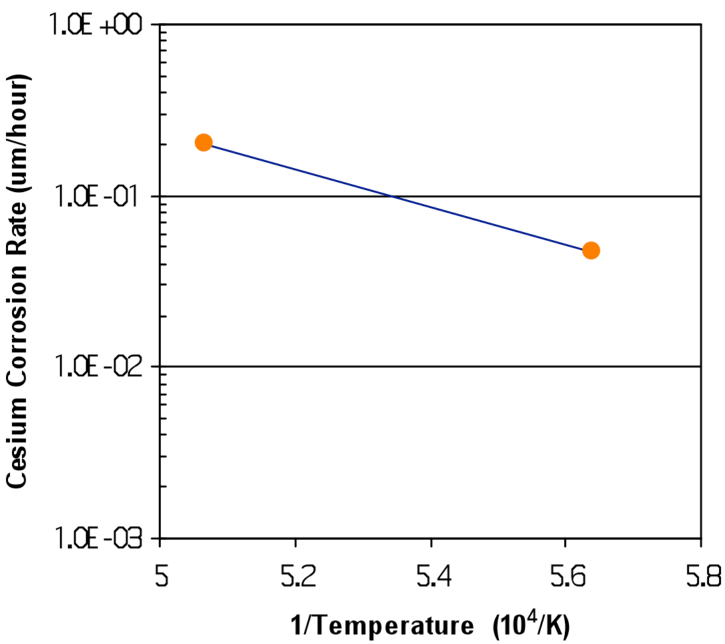


500:1

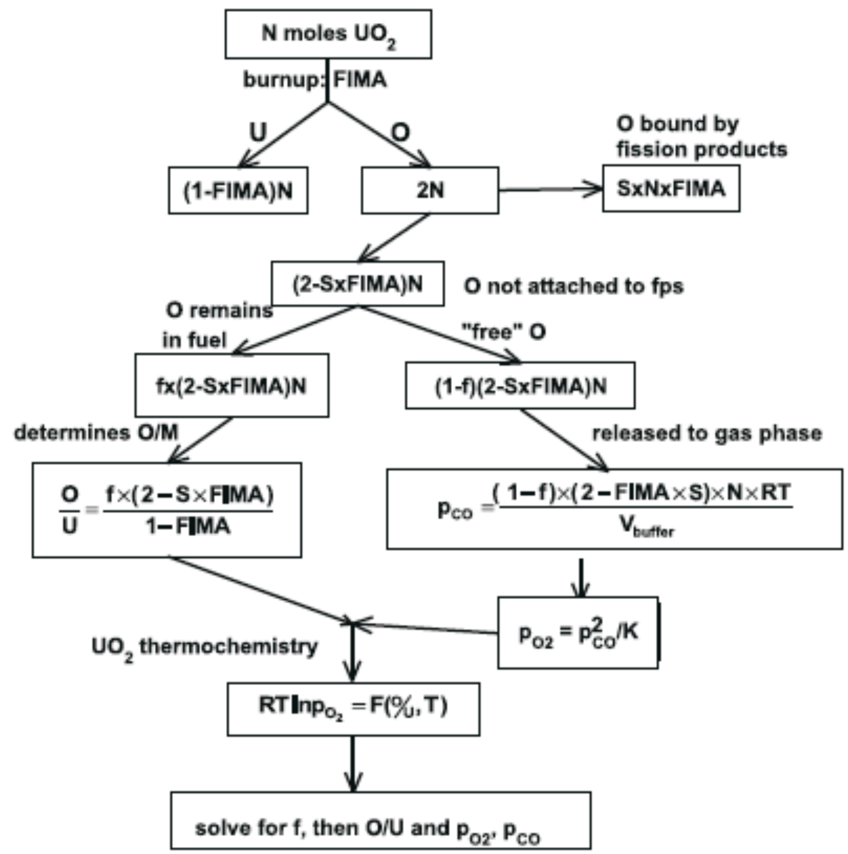
Cesium Degradation of the SiC Layer

- Older data from ISPRA (Coen et al.) exposed SiC to cesium vapor. Degradation/interaction was observed at both cases
  - 85 hrs at 1500°C and 2500 Pa --> 3.5 to 5 micron penetration
  - 198 hrs at 1700°C and 12800 Pa --> 40 micron penetration.
- Hard to determine if there is a pressure dependence to this interaction
- Currently funding new experiments under NEUP



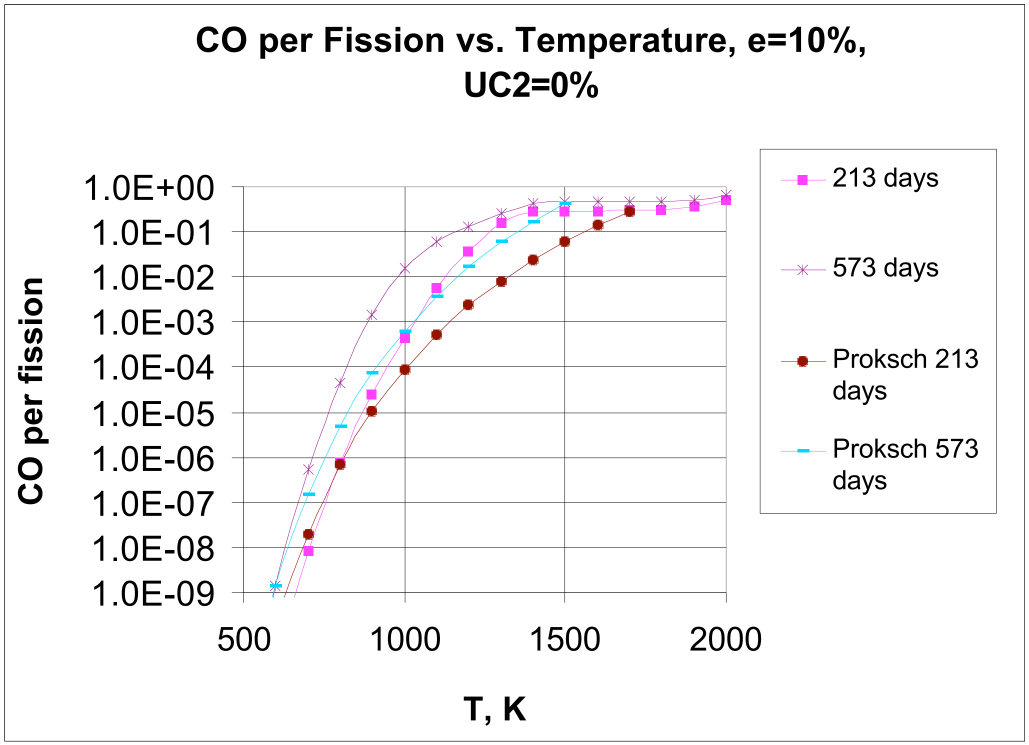
CO production: UO_2 vs. UCO

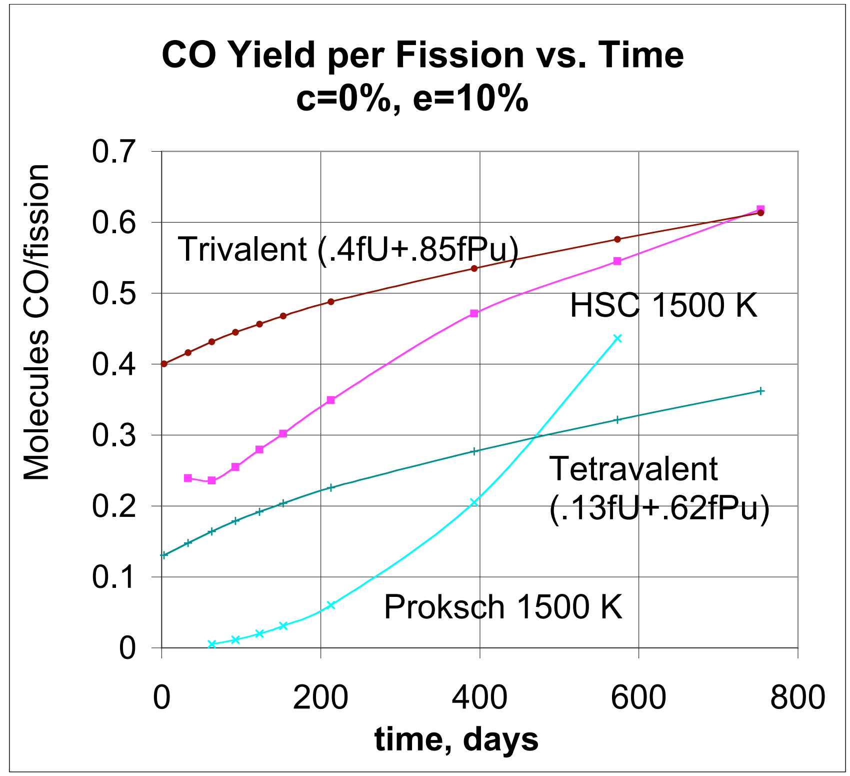
- The release of excess oxygen by fission in UO_2 fuels causes CO production to become significant at high burnup and accident temperatures
  - Fission produces 2 oxygen atoms
  - Fission products react with about 1.6 oxygen atoms per fission
  - 0.4 excess oxygen atoms react with carbon to form CO
- In UCO, enough uranium carbide is added to react with the oxygen so no CO is produced



The release of excess oxygen in UO_2 fuels causes CO production to become significant at high burnup

Comparisons of new INL model with German correlation (600 days =~ 5% FIMA)
Data underlying German correlation show large scatter. There are no data for high burnup fuel





CO Degradation of the SiC Layer

- Beyond the pressure increase, it is known that CO will interact with SiC via the reaction at high temperatures
  - CO + SiC <--> SiO + C
- This has been a concern in the event of a cracked IPyC since the CO could directly attack the SiC layer
- However, there is evidence from the surface science literature suggests that CO can intercalate in the carbon layer.
- If CO can intercalate during normal operation it could subsequently permeate through the IPyC layer at high temperatures albeit perhaps in small amounts and react with SiC. Since SiO is a gas, the chemical attack would look like a degradation probably starting at the grain boundaries and leave no “visible” trace.
- Given the potential for high CO production at high burnups in LEU UO_2, this may become increasingly more important.
- Currently funding experiments in this area under NEUP

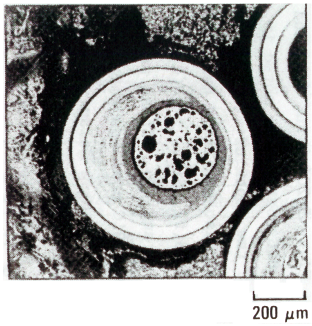
Kernel Migration or Amoeba Effect

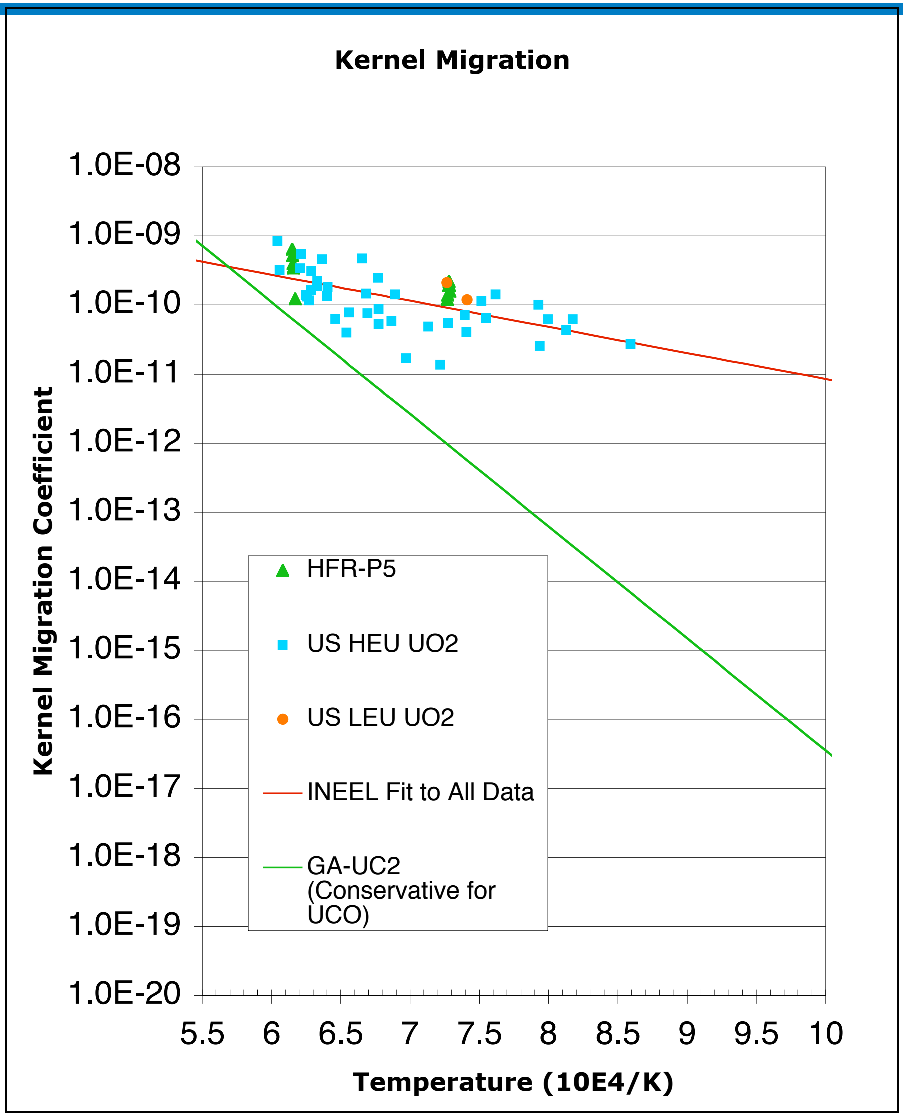
- Migration in a temperature gradient to the hot side
- Depends on temperature gradient and temperature

$$\vec{\delta}_{MIG} = \int KMC \bullet \frac{\vec{\nabla T}}{T^2} d\tau$$

$$KMC = KMC_O * \exp(-Q/RT)$$

- Data exist for UO_2, ThO_2,$(U,Th)O_2$, and UC_2: both HEU and LEU





Experimental Database and Reactor Implications

- Kernel migration, the tendency of UO_2 to migrate up the thermal gradient has been observed in many irradiation experiments

Capsule	Max. Avg. Temp.	UO2 Peak Burnup (%FIMA)	Kernel Migration	Max. Avg. Temp.	UCO Peak Burnup (%FIMA)	Kernel Migration
HRB-14	1070°C	29.5	16 μm	1100°C	28.6	none
HRB-15A	1125°C	28.5%	≤ 30 μm in 22%	1110°C	25	none
HRB-16	1150°C	27.8	20-55 μm	1105°C	27	none

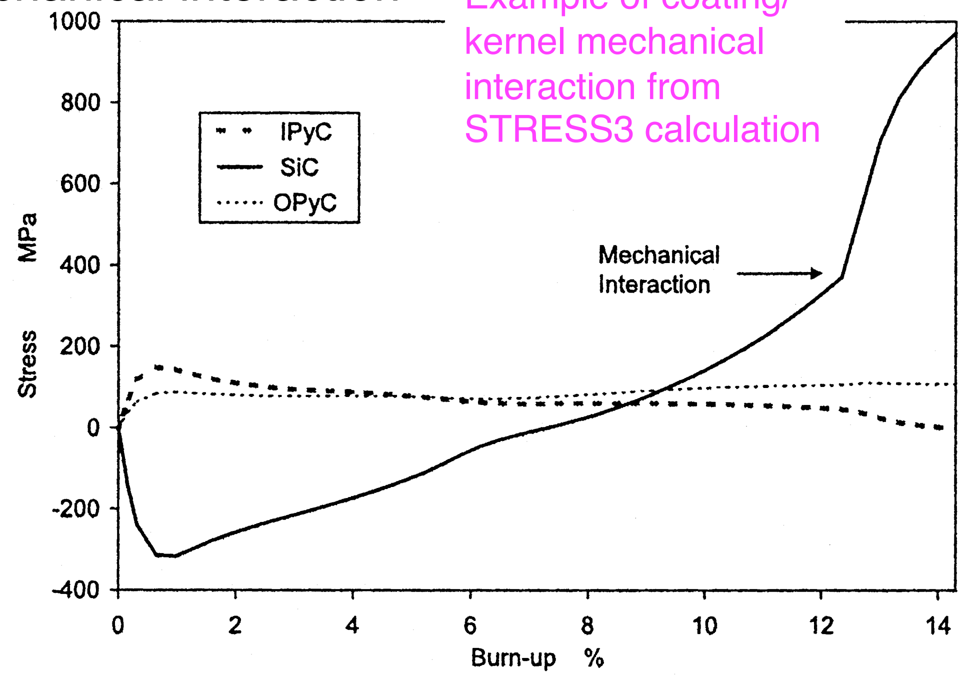
Data provided by GA

- The impact for a given reactor design depends on irradiation conditions
  - Not a problem in the German pebble bed (AVR) because of low power density and circulating fuel
  - Was a problem in large HTGR designs
  - Need an NGNP design to evaluate impact however, at high core power densities expected for NGNP, which typically occur in prismatic cores and near inner reflectors, kernel migration could occur

Solid Fission Product Fuel Swelling is Important at High Burnup

- Theoretical estimates (Olander) of swelling range from 0.3 to 0.45% ΔV/V per atom percent burnup.
- Experimental measurements suggest even larger values 0.6-1.5% Δ V/V per atom percent burnup (probably due to intergranular fission gas bubbles)
- At 20% FIMA, this corresponds to 6 to 30% increase in volume of kernel
- Large amount of swelling can reduce void volume in particle and under some conditions cause kernel/coating mechanical interaction
  - Buffer layer tends to show largest distribution in thickness because of speed of coating.
  - Monte Carlo simulations suggest that large fraction of buffers with thin coatings are subject to this potential interaction
  - Particle redesign (thicker buffer or reduced variation in thickness) may help ameliorate this concern.

Example of coating/ kernel mechanical interaction from STRESS3 calculation



Overview of Approach for Particle Fuel Performance Modeling

Fracture Strength Comparison of PyC and SiC

Weibull theory is used to predict failure of each layer

$$P_f = 1 - e^{-\int_V (\sigma/\sigma_0)^m dV}$$

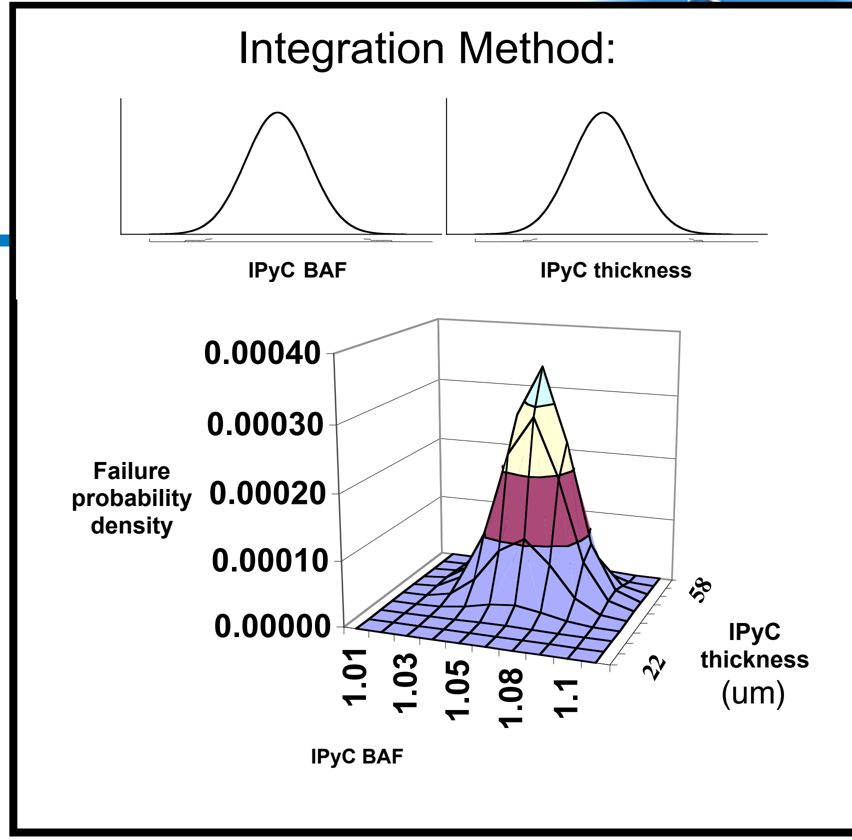
$$P_f = 1 - e^{-(\sigma_c/\sigma_{ms})^m}$$

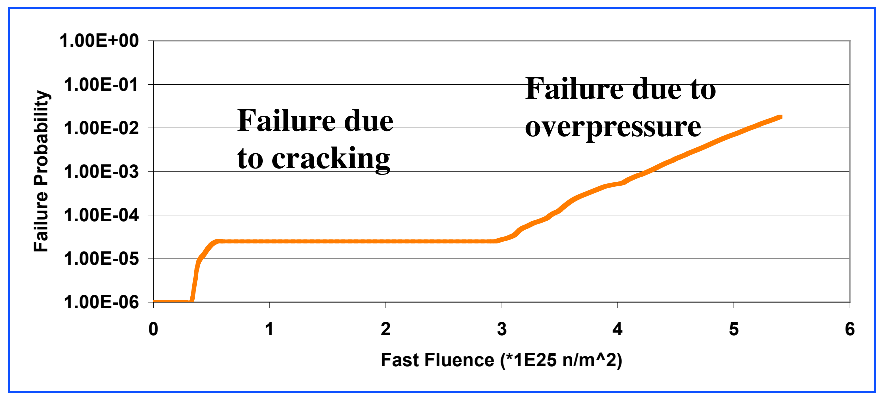
- PyC
  - GA value σ_m = 300 MPa m= 9.5 σ(1e-04) = 114 MPa
  - German σ_m ~ 200 MPa m= 5 σ(1e-04) = 34 MPa
- SiC
  - GA value σ_m = 500 MPa m= 6 σ(1e-04) = 107 MPa
  - STAPLE(UK) σ_m = 200 MPa m= 5 σ(1e-04) = 34 MPa
  - German (unirrad.) σ_m = 834 MPa m= 8 σ(1e-04) = 276 MPa
  - German (irrad.) σ_m = 687 MPa m= 6 σ(1e-04) = 157 MPa
- Values are determined by flaw distribution in the material and volume of the layer

Determination of Failure Probability

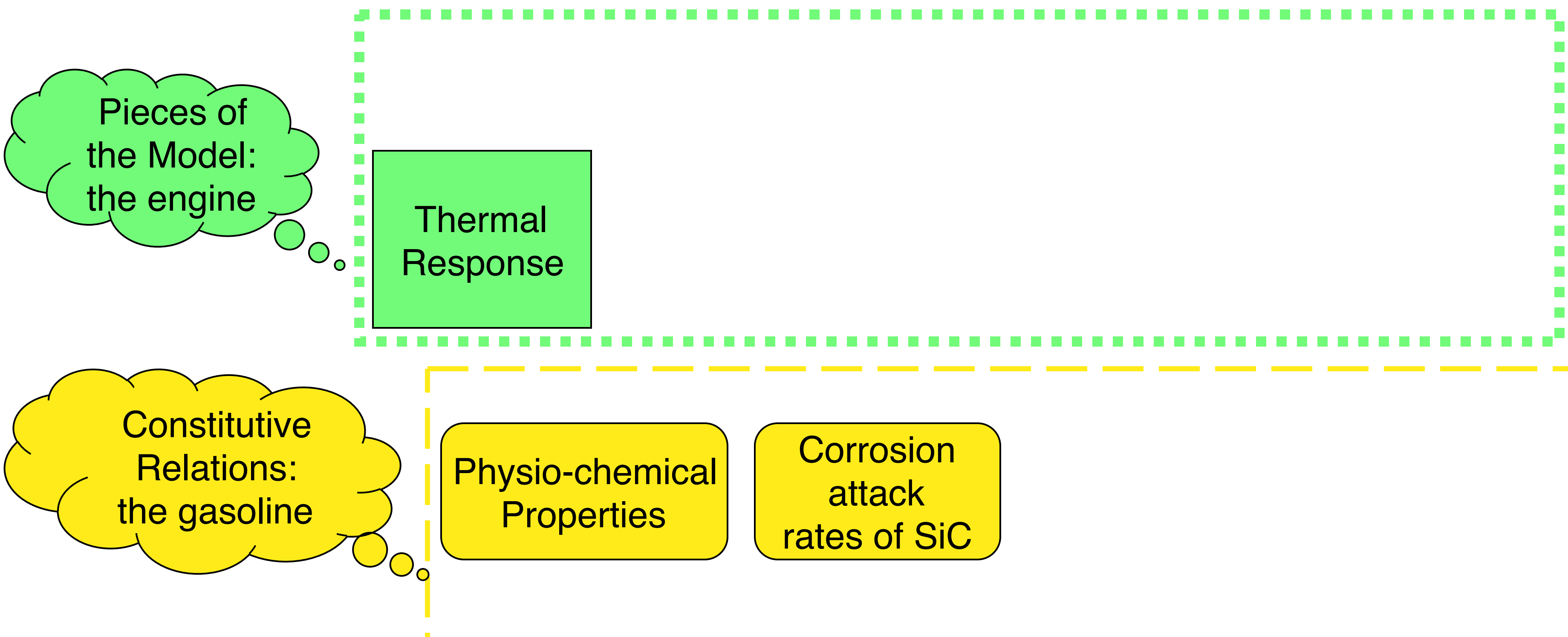
Results from finite element analyses on multi-dimensional particles are used in conjunction with results from a one-dimensional solution to estimate stresses in any random particle

- *Monte Carlo (MC) method – statistically samples a large population of particles considering statistical variations among particles*
- *Integration approach – integrates failure probability over parameter space, considering the same statistical variations*
  - *Can be much faster tha n MC, depending on how many parameters are varied*
  - *Serves to verify MC results and vice versa*
- *Conceptually the two methods give identical results when the sample size for the MC method is large, then MC takes longer and integration method is more efficient*





Overview of Approach for Particle Fuel Performance Modeling



PARFUME Thermal Models: Fuel Element and Fuel Particle

- For the macro-temperature field in fuel element
  - Pebble or cylinder
- For the particle

$$\rho c \frac{\partial T}{\partial t} = k \frac{\partial}{\partial x}\left(\frac{\partial T}{\partial x}\right) + q'$$

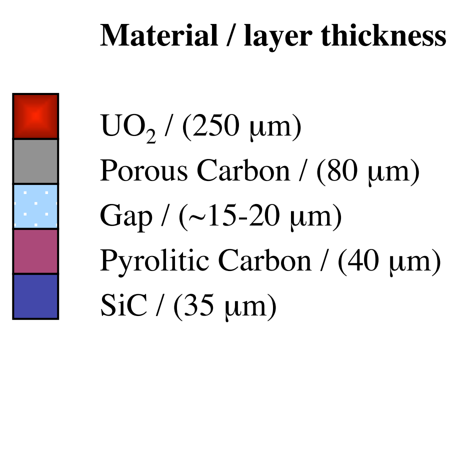
$$\rho c \frac{\partial T}{\partial t} = \frac{k}{r} \frac{\partial}{\partial r}\left(r \frac{\partial T}{\partial r}\right) + q'$$

and

$$\rho c \frac{\partial T}{\partial t} = \frac{k}{r^2} \frac{\partial}{\partial r}\left(r^2 \frac{\partial T}{\partial r}\right) + q'$$

$$\frac{\partial T}{\partial t} = \alpha \left\{ \frac{1}{r^2} \frac{\partial}{\partial r}\left(r^2 \frac{\partial T}{\partial r}\right) + \frac{1}{r^2 \sin\theta} \frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial T}{\partial \theta}\right) + \frac{1}{r^2 \sin^2\theta} \frac{\partial^2 T}{\partial \phi^2} \right\} + \frac{q'}{\rho c}$$

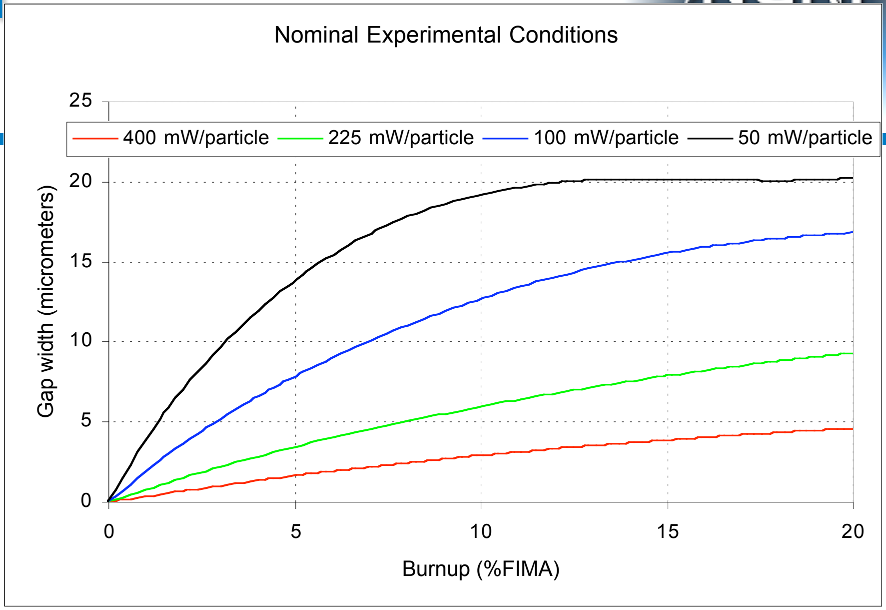
Thermal Behavior in Coated Particle

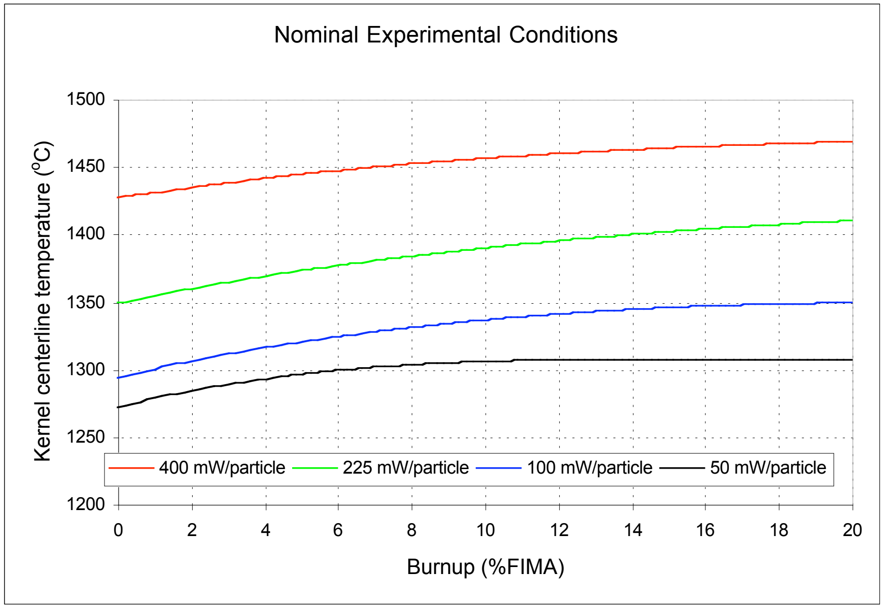


- Key thermal resistance is the gap that develops as buffer shrinks under irradiation, increasing with neutron fluence (dose)
- The gap fills with fission gas and CO (for UO_2) and the mixture is a function of burnup
- Thermomechanical response of the buffer and the resulting gap size depends on the boundary conditions (restrained vs. unrestrained buffer)
- Peak kernel temperature is thus a function of burnup, fluence and power per particle

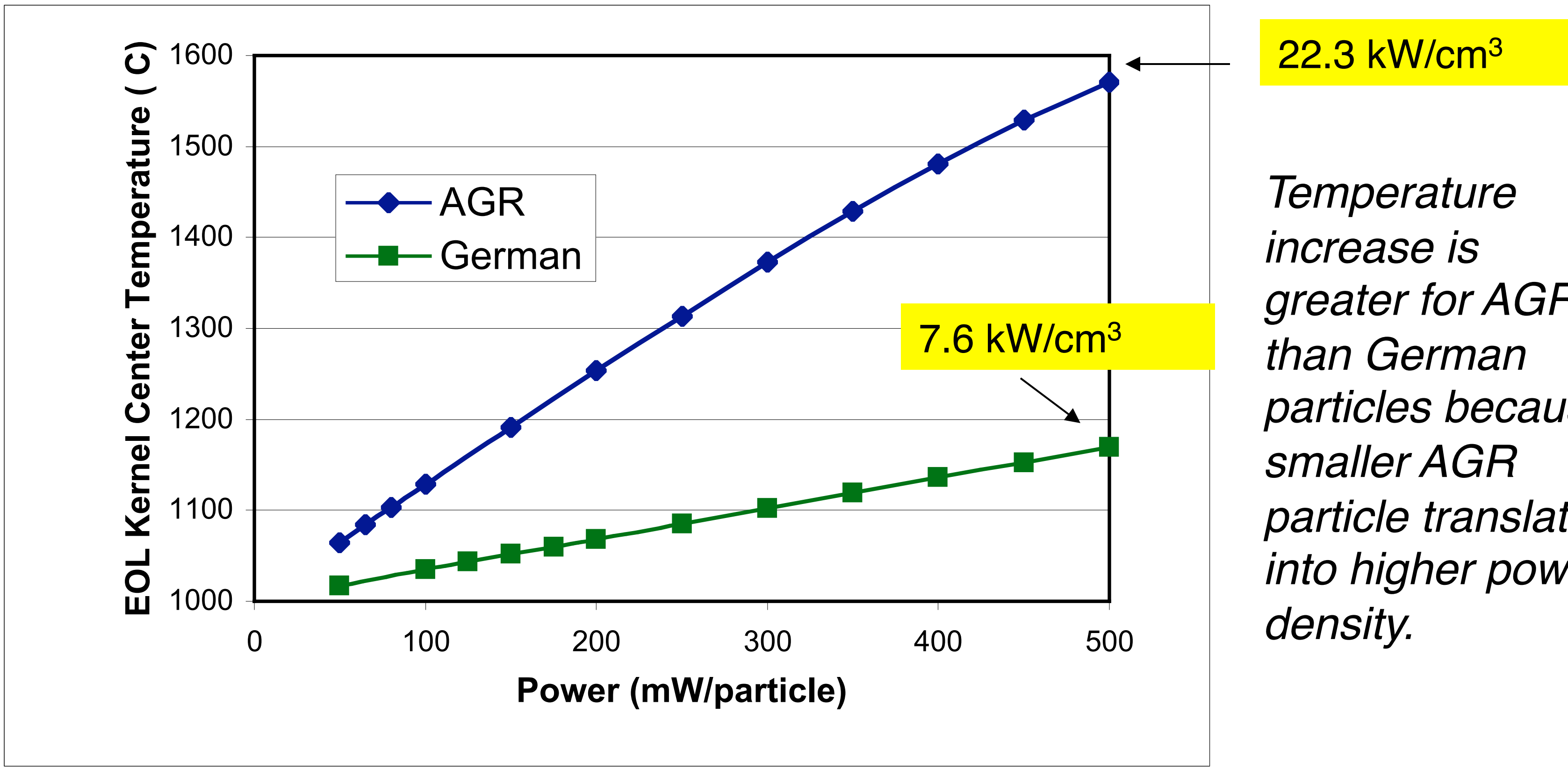
Particle behavior in irradiation as a function of burnup and power in AGR-1

- Gap grows with fluence and is filled with fission gas as burnup increases
- Very high kernel temperatures seen for high powers
- AGR-1 expected to remain below 200 mW/particle
- Volume average temperature of compact is 1250°C (outside OPyC temperature)
- Lower power particles take longer time to reach peak burnup and thus acquire greatest fast fluence





Kernel center temperature increases because of increasing thermal resistance provided by gap between buffer and IPyC filling with noble gases and CO and because of increasing power.



Temperature increase is greater for AGR than German particles because smaller AGR particle translates into higher power density.

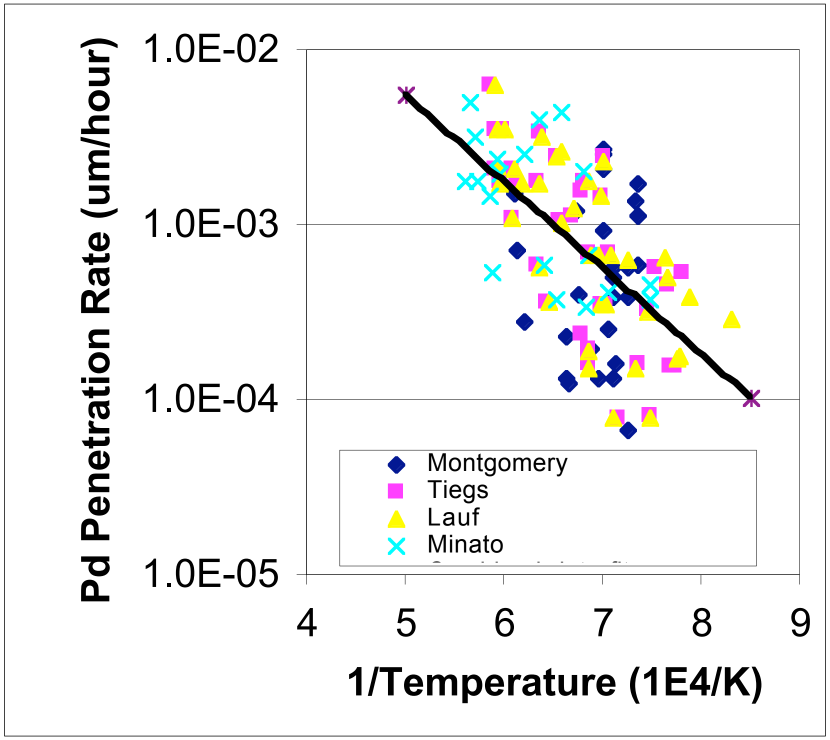
PARFUME calculates that ~ 20 micron gap develops in each particle because of dimensional changes in buffer and IPyC and kernel swelling.

High burnup behavior of LEU coated particle fuels: Ag and Pd

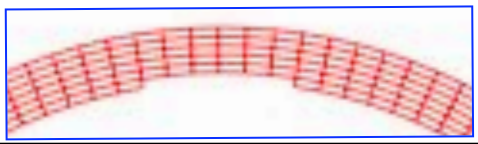
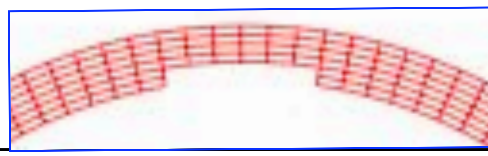
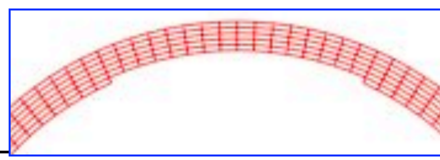
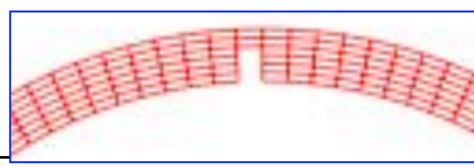
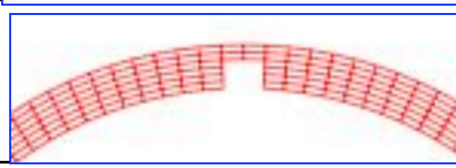
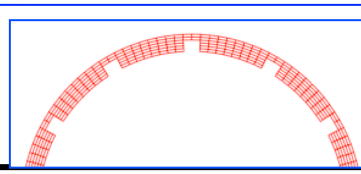
- With high burnup LEU, 25 to 50x more Ag and Pd are produced than in either HEU or LEU low burnup fuels because of the large fraction of fissions from Pu that are expected at high burnup.
- Could result in greater Ag release and higher potential for Pd attack of the SiC
- Ag release may be as a result of Knudsen diffusion via nano-sized passages (cracks, pores). Unclear if this can be remedied in the fuel per se
- Data from postirradiation examination will provide estimates of the magnitude of the problem
- Available in-pile data suggest that Pd attack on the SiC is a function of temperature. The number of attack sites at the SiC is a weak function of the Pd concentration. No direct correlation with burnup or fast fluence
- Accident heatup testing of high burnup LEU fuel compacts will determine if Pd attack is a problem for NGNP

Pd Interactions in SiC

- Pd/SiC interactions have been the subject of extensive study. Reviewed international historical database
- Selected irradiation data from UO_2 with some UC_2. (both irradiation capsules and FSV data)
- Temperatures from ~ 950 to 1550°C
- No concentration (burnup) or kernel composition dependence observed
- Arrhenius temperature dependence. Activation energy of ~ 94 kcal/mole

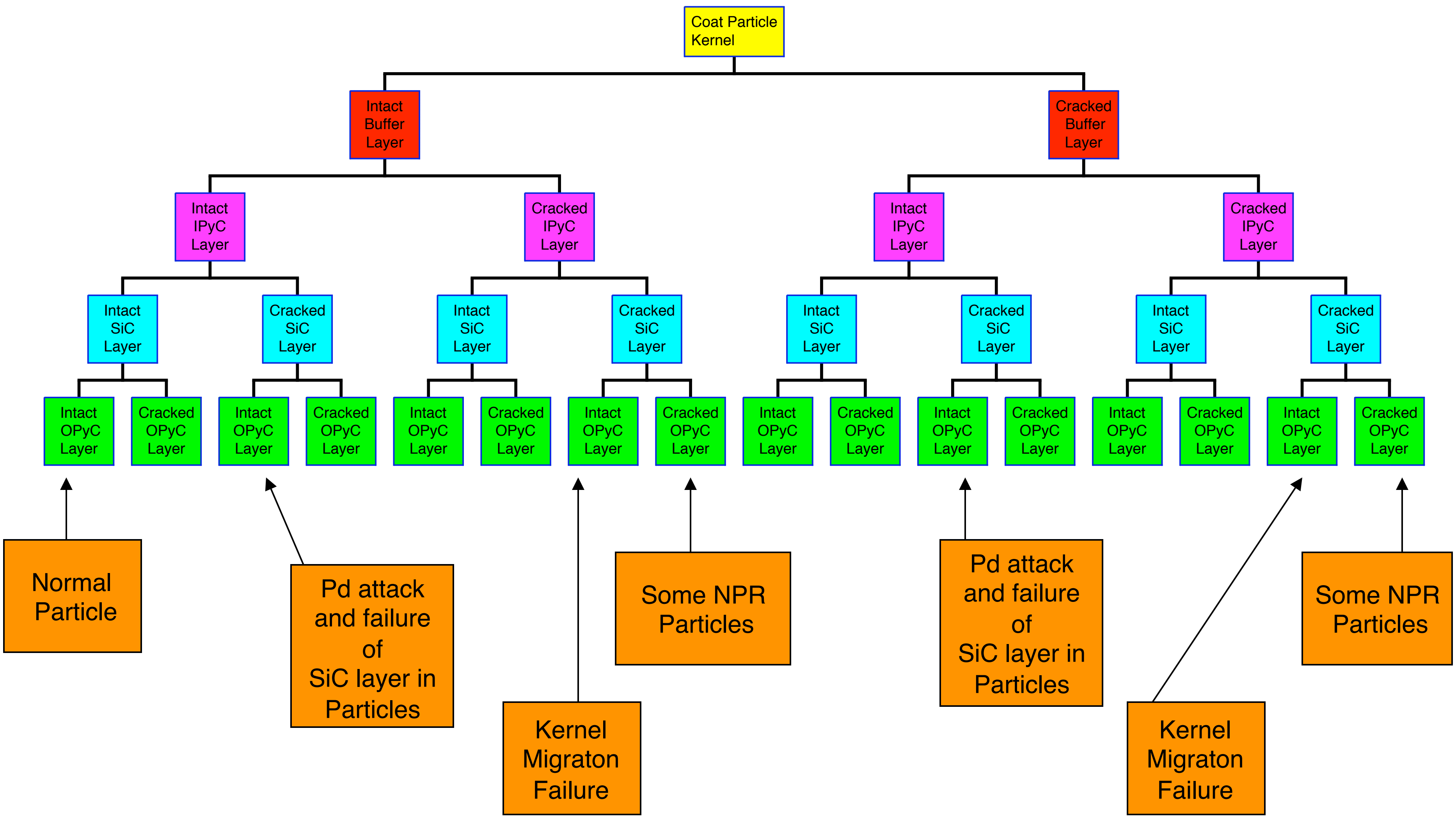


Defining Particle Failure from Pd Attack using finite element structural analysis using different reaction zone shapes

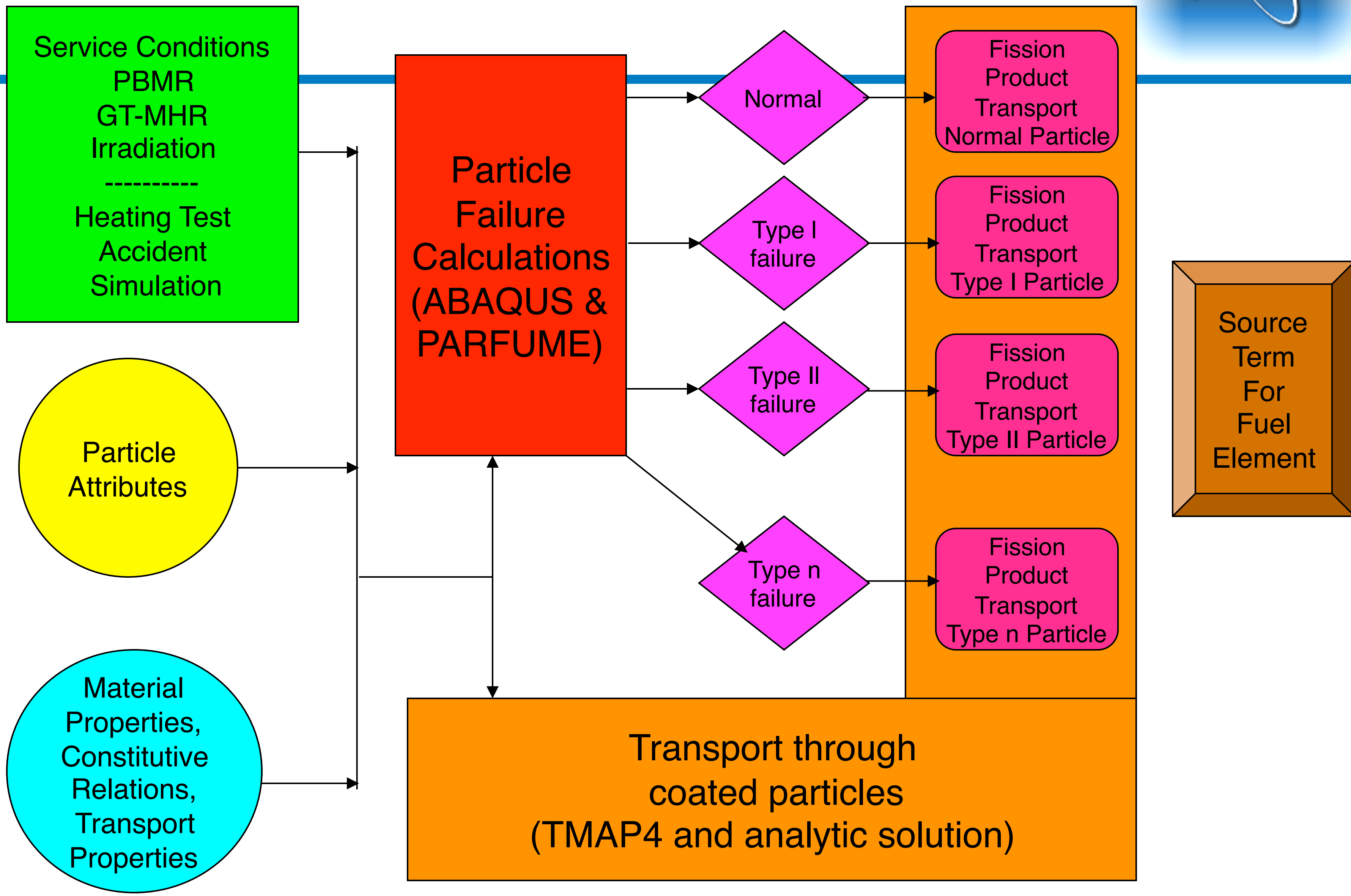
Reaction Zone Type	Finite Element Model	Size of Zone (µm x µm)	Calculated Failure Probability
Base - 1		5.8 × 104	1.78×10^{-4}
Base - 2		11.7 × 104	3.00×10^{-4}
Very Wide		5.8 × 279	1.62×10^{-3}
Narrow - 1		23.3 × 17.4	9.38×10^{-6}
Narrow - 2		23.3 × 34.8	2.65×10^{-5}
Multiple		23.3 × 34.8 5 places	9.7×10^{-5}

Overview of Approach for Particle Fuel Performance Modeling

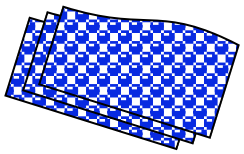
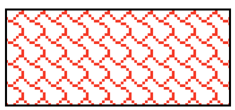
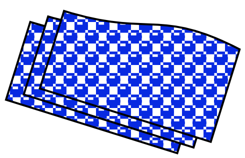
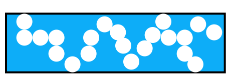
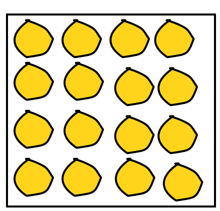
Potential Configurations of particles for fission product transport calculations



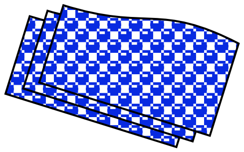
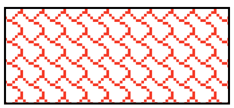
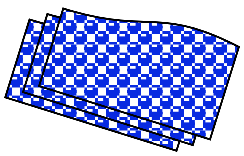
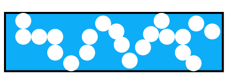
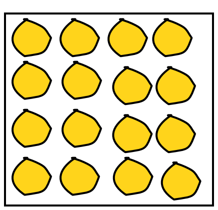
Source Term Calculation Flowchart



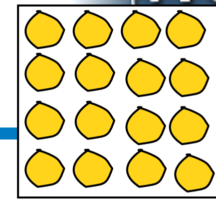
Thoughts on Fission Product Modeling and Mechanisms: Gases

		Structure	Gases: Kr,Xe, Ag
OPyC		Same as IPyC	Much slower Knudsen diffusion through the small amount of porosity. Need to know interconnected porosity and tortuosity of the material.
SiC		Polycrystalline small grained structure	Slower Knudsen diffusion through any porosity and or defects in the layer. Need to know interconnected porosity and tortuosity of the material. Bulk diffusion may become important at high temperature
IPyC		High density layered carbon structure	Much slower Knudsen diffusion through the small amount of porosity. Need to know interconnected porosity and tortuosity of the material. At high temperature, bulk diffusion may also be important.
Buffer		Porous carbon	Rapid Knudsen diffusion through the porosity
Kernel		Ceramic collection of grains and grain boundaries	Diffusional transport of atoms and bubbles from the grains to the grain boundaries. When grain boundaries interconnect, large release. Booth equivalent sphere model is used and well accepted.

Thoughts on Fission Product Modeling and Mechanisms: Condensible FPs

		Structure	Condensible:Cs, Sr, Pd (?)
OPyC		Same as IPyC	Same as OPyC however trapping and intercallation effects may be more important given the lower concentration of fission products expected in this layer compared to IPyC.
SiC		Polycrystalline small grained structure	Most likely grain boundary diffusion is operable at low temperatures. Bulk diffusion may become important at high temperature. Need to know the area fraction occupied by grains and boundaries and individual diffusivities of the boundary and the bulk to set up a parallel path diffusion model. Can be done in TMAP.
IPyC		High density layered carbon structure	Elements like Cs will intercalate in between the layers. Transport is a diffusion and trapping type mechanism, probably along the edges of the carbon grains. Need to understand the nature of the chemical bonding and the details of the microstructure. At high temperature, bulk diffusion may also become important.
Buffer		Porous carbon	Rapid diffusion through the porosity
Kernel		Ceramic collection of grains and grain boundaries	Diffusional transport of atoms to the grain boundaries. Grain boundary diffusion to the surface.

Modeling the Kernel



- Booth equivalent model is the basis for models historically used by both gas reactor and LWR fuel modelers to describe fission product release
  - No explicit account for changes with burnup. Effective diffusivities can be used to incorporate complex phenomena in a simple way
  - Fractional release

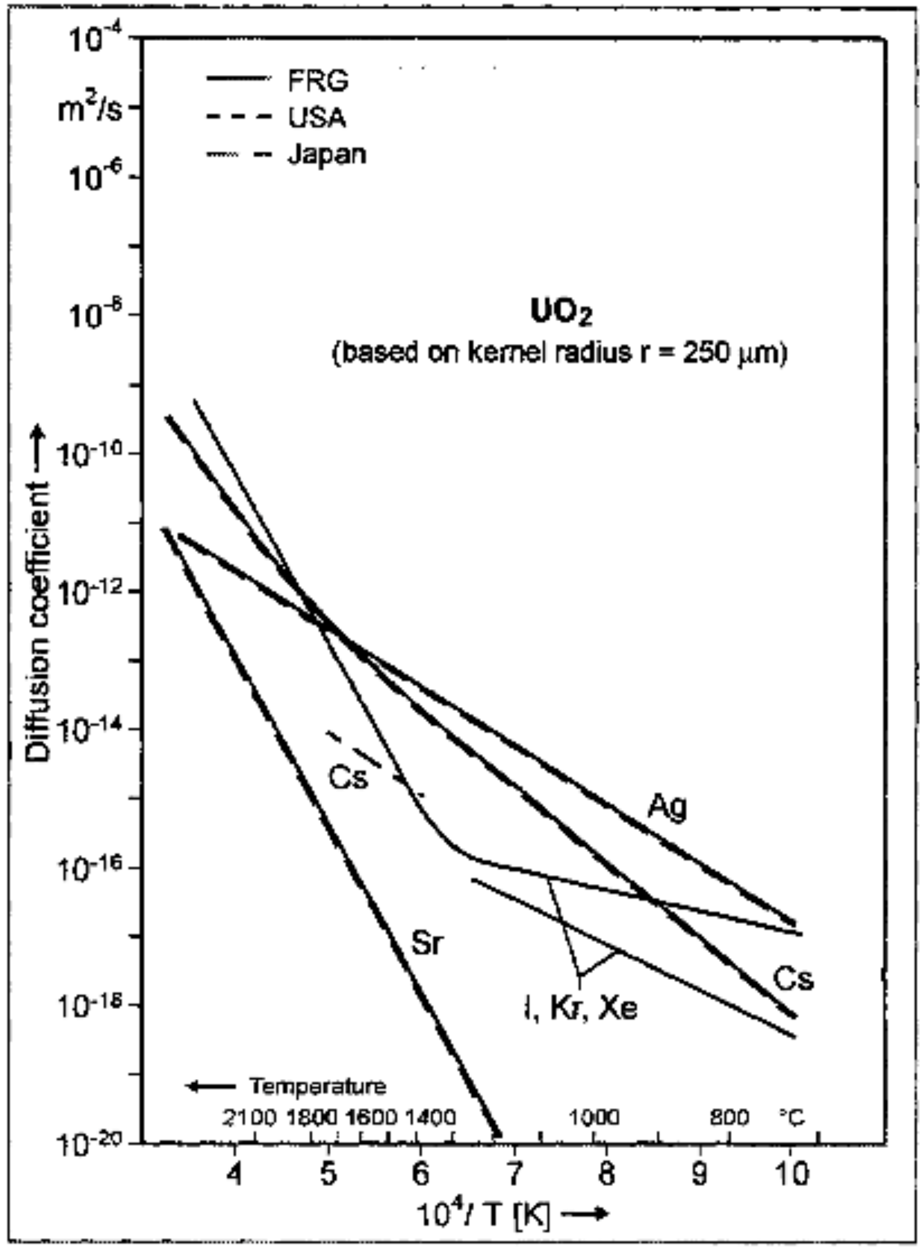
$$FR = 1 - \left(\frac{6}{D' t}\right) \sum_{n=1}^{\infty} [1 - \exp(-n^2 \pi^2 D' t)] / [n^4 \pi^4]$$

  where $D' = D/a^2$

  - For UO_2
    - $D_{gas} = D_{intrinsic} + D_{athermal} + D_{rad\ enhanced}$
    - $D_{effective}$ exists for Cs, Ag, and Sr
  - For UCO, there are little data. Values for UO_2 are usually used

Effective Diffusion Coefficients in UO_2

(from IAEA Tecdoc)



Complete fission gas release is expected at high burnup in both UO_2 and UCO

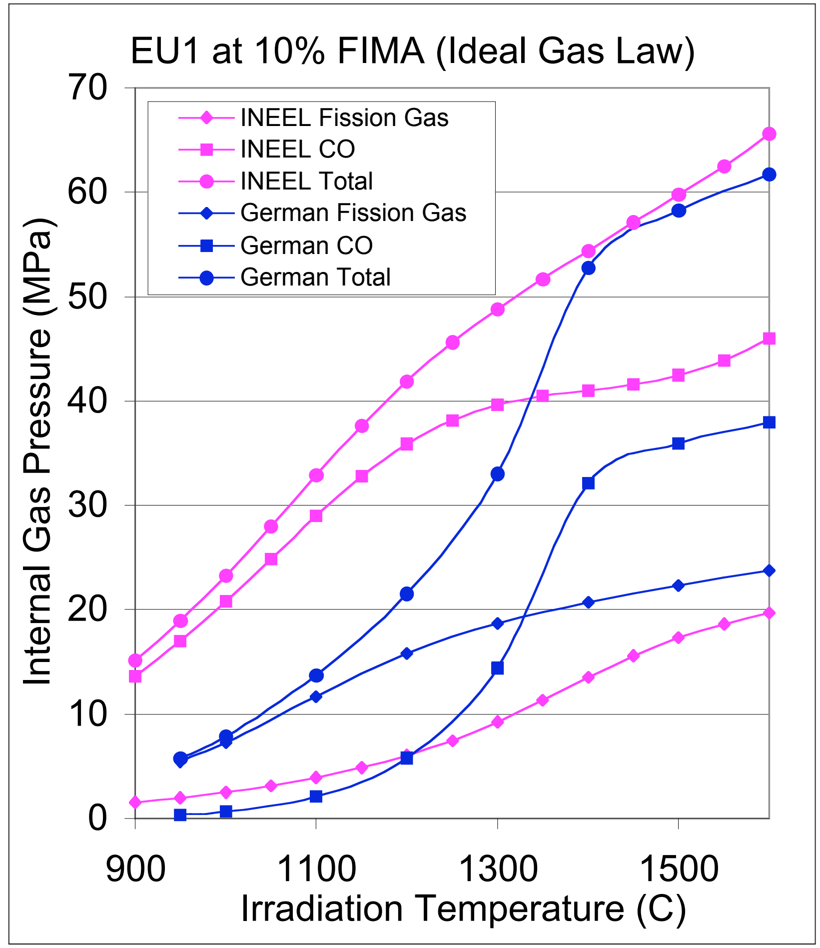
- Large amount of data available for UO_2 from LWR experience
- Gas in the fuel kernels migrate to grain boundaries and form bubbles. Release is determined by time at temperature.
- These bubbles form an interconnected porosity and are released from the kernel at higher burnups
- German, US and UK models use the classic Booth equivalent sphere diffusion model. Differences in the diffusivity values used.
- Impact on results in terms of fractional release of gas from the kernel is fairly small under gas reactor conditions at high burnup

Fission Gas Release Fraction

	German Fuel	US HEU (NPR)
Burnup/Temp./Time	(8.5% FIMA/1173 K/3yr)	(79% FIMA/1473K/3 yr)
PARFUME (US)	.23	.86
MINIPAT (UK)	.33	.95

Comparison of Gas Pressure Results

- Fission gas release - Equivalent Booth Equivalent Sphere Model; Diffusivities based on Turnbull
- CO production based on thermodynamic calculations as function of burnup, temperature, enrichment and fuel composition (O/U, C/U)



Modeling Knudsen and Pressure Driven Diffusion: Gases

Kn>1 free molecular flow

$$\dot{N}_{Kn} = -\frac{D_{Kn}}{RT}\frac{\varepsilon_p}{\mu_{p,Kn}}\nabla p$$

$$D_{Kn} = (4/3)\,\bar{d}_{pore}\sqrt{RT/2\pi M}$$

Kn < 0.01 continuum region

$$\dot{N} = \dot{N}_{vis} + \dot{N}_{diff}$$

$$\dot{N}_{diff} = -\frac{D_{12gas}}{RT}\frac{\varepsilon_p}{\mu_{p,Dif}}\nabla p$$

0.01 < Kn < 1 transition region

$$\dot{N} = \dot{N}_{vis} + \dot{N}_{diff}$$

$$\dot{N}_{diff} = -\frac{D_{Eff}}{RT}\frac{\varepsilon_p}{\mu_{p,Kn}}\nabla p$$

$$D_{Eff} = \left[\frac{1}{D_{Kn}} + \frac{1}{D_{12gas}}\right]^{-1}$$

$$D_{Kn} = (4/3)\,\bar{d}_{pore}\sqrt{RT/2\pi M}$$

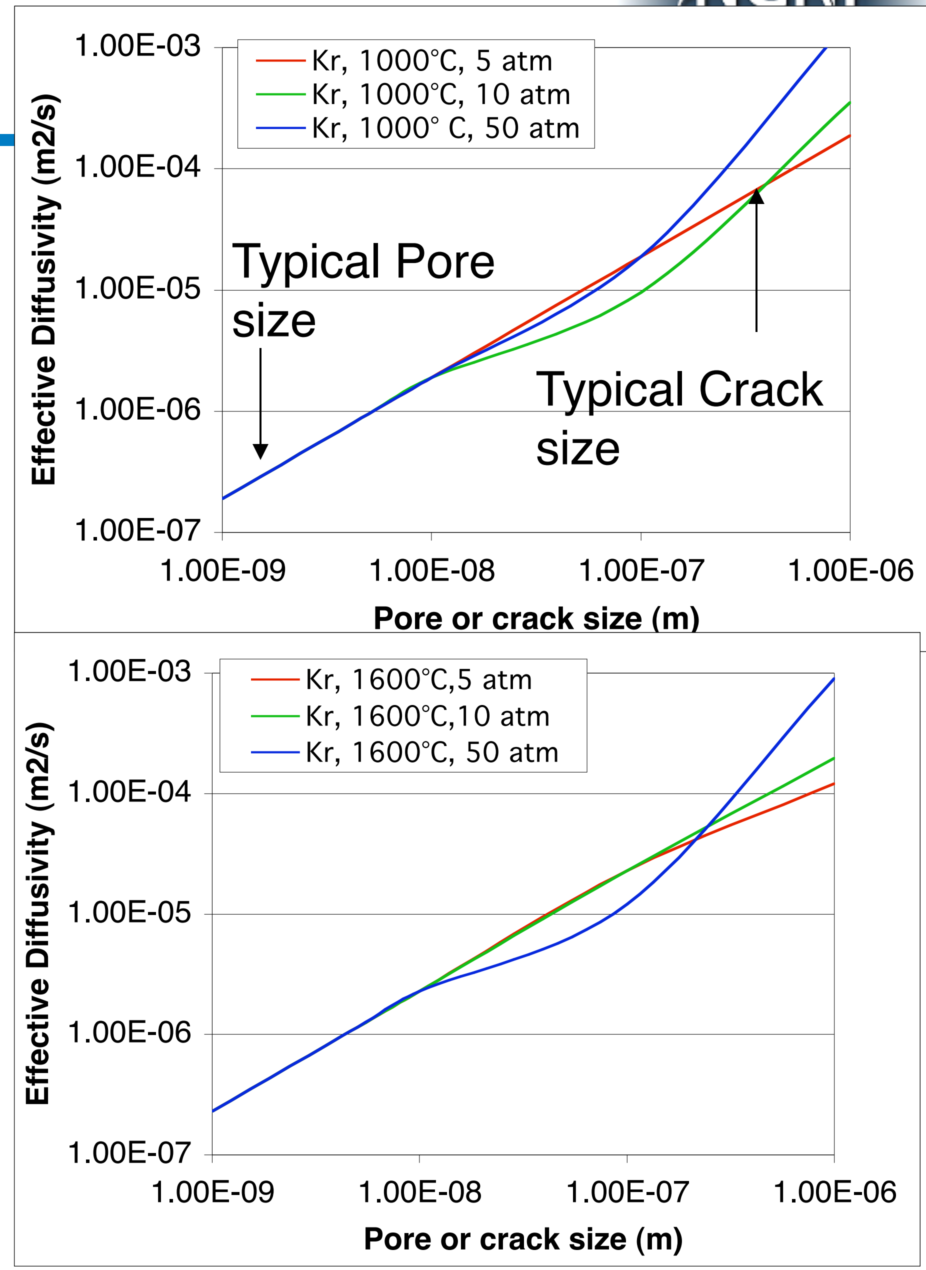
$$D_{12gas} = Chapman - Eskong - Theory$$

$$\dot{N}_{visc} = -\frac{k\,\bar{p}}{\eta RT}\nabla p$$

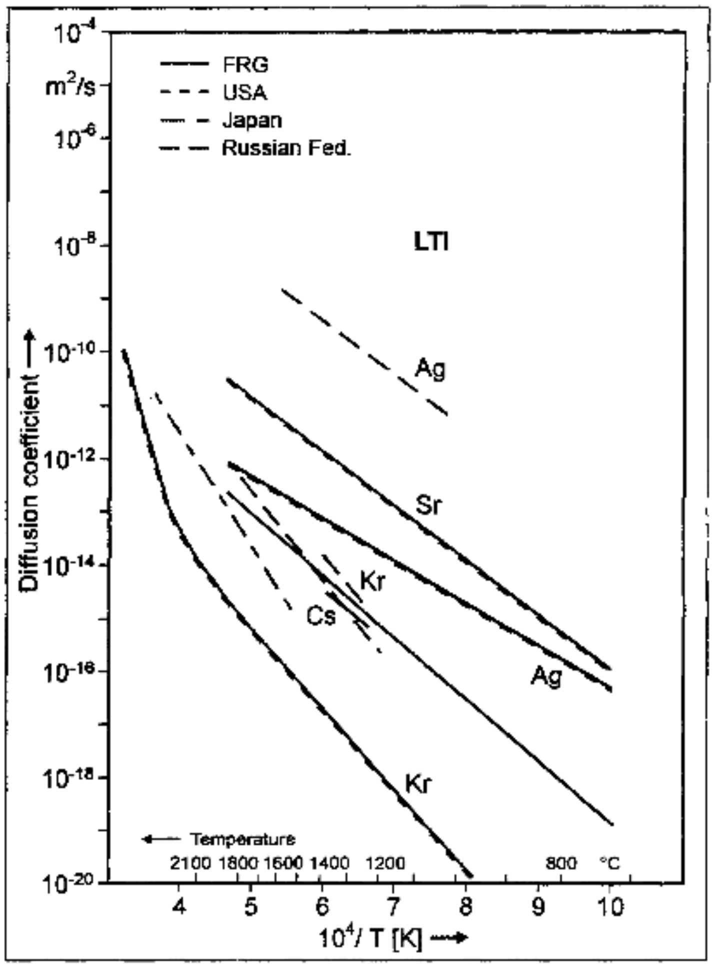
- Depends on Kn number
- Need to know pore size, porosity, and tortuosity of the PyC

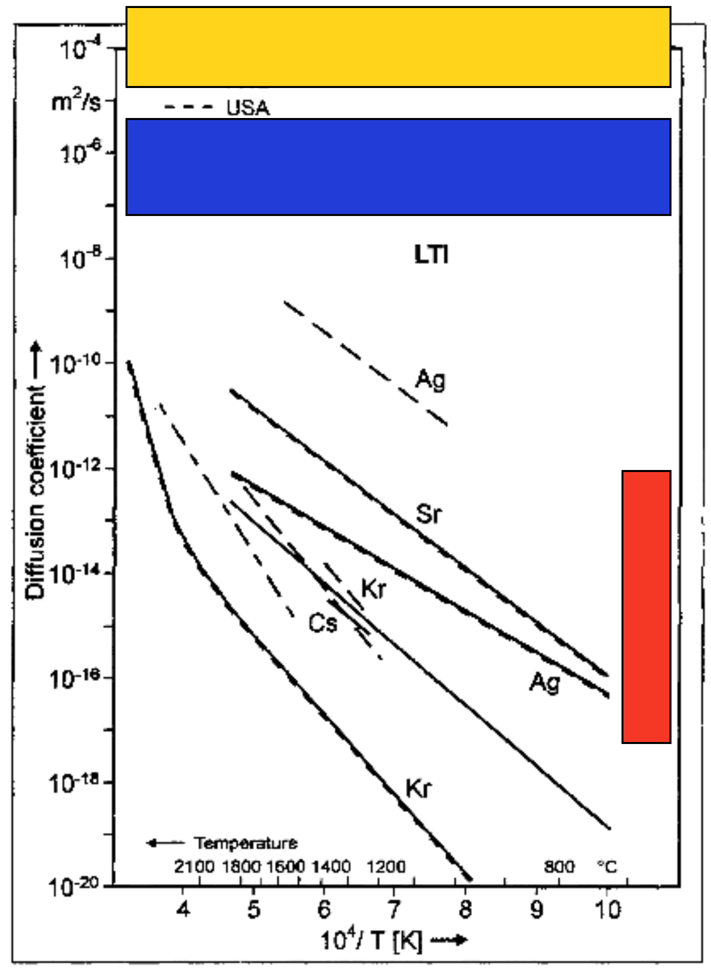
Gas Phase Transport Results for Gases

- Transport through nanopores, D_{Kn}~2 to 3×10^{-7} m^2/s
- Transport through cracks (~1 micron), D ~ 10^{-4} to10^{-3} m^2/s
- Such rapid transport is typical of buffer but does not fit with measured effective diffusivities in PyC and SiC



Effective Diffusion Coefficients through PyC (from IAEA Tecdoc)





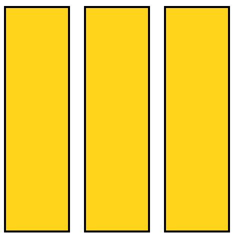
Knudsen diffusion through nanopores

Viscous diffusion through microcracks

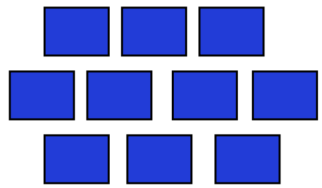
Older permeability estimates of CO_2 and He on PyC

Influence of Microstructure

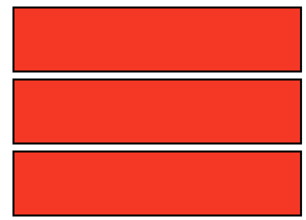
Account for multiple grains and their random orientation



Idealized large columnar structure



Small grain structure



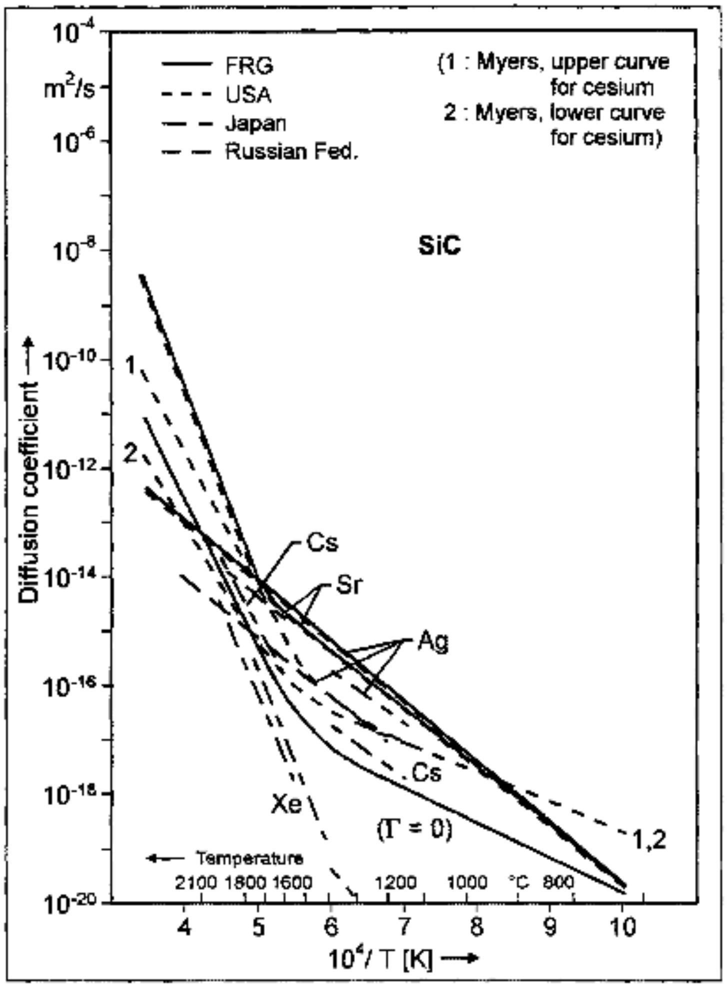
Idealized laminar structure

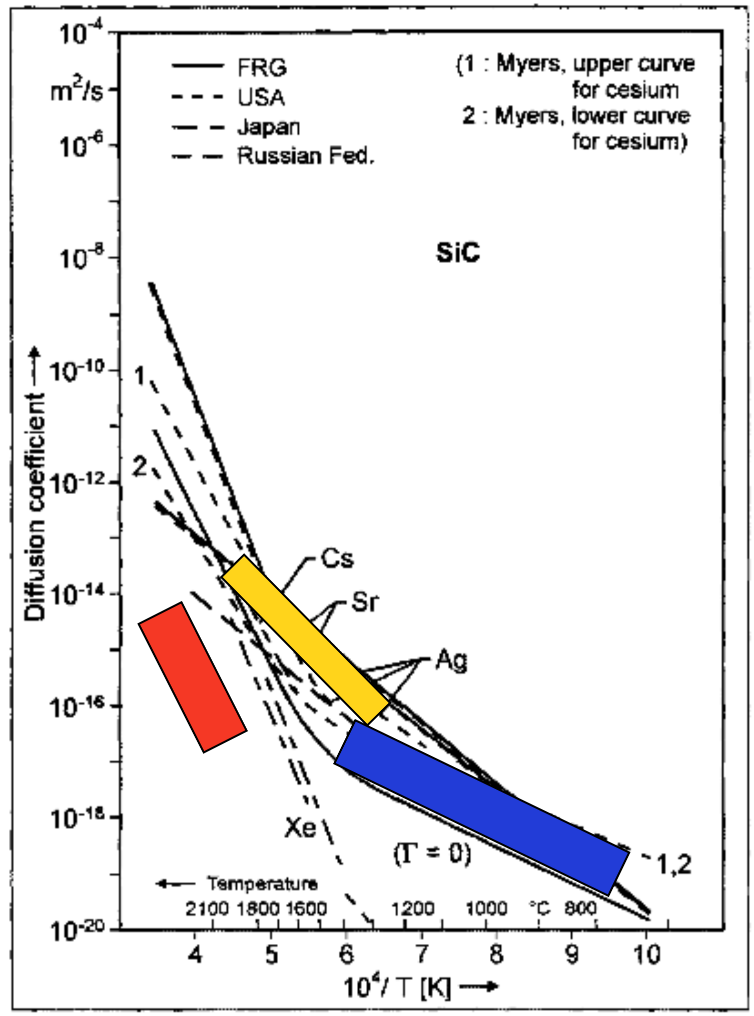
$$D_{eff} = D_v(1-f) + D_{gb}f$$

$$D_{eff} = \frac{D_v D_{gb}}{D_v(1-f) + D_{gb}f}$$

These two mixture rules will bound behavior of small crystal SiC

Effective Diffusion Coefficients through SiC (from IAEA Tecdoc)

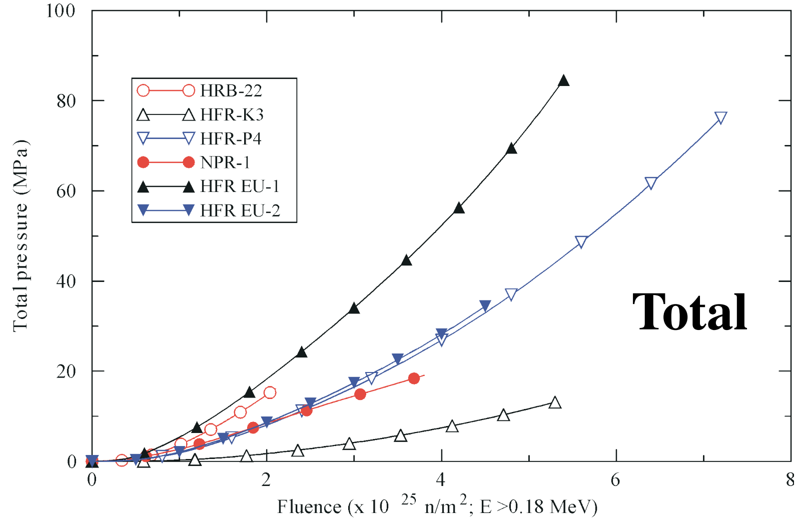


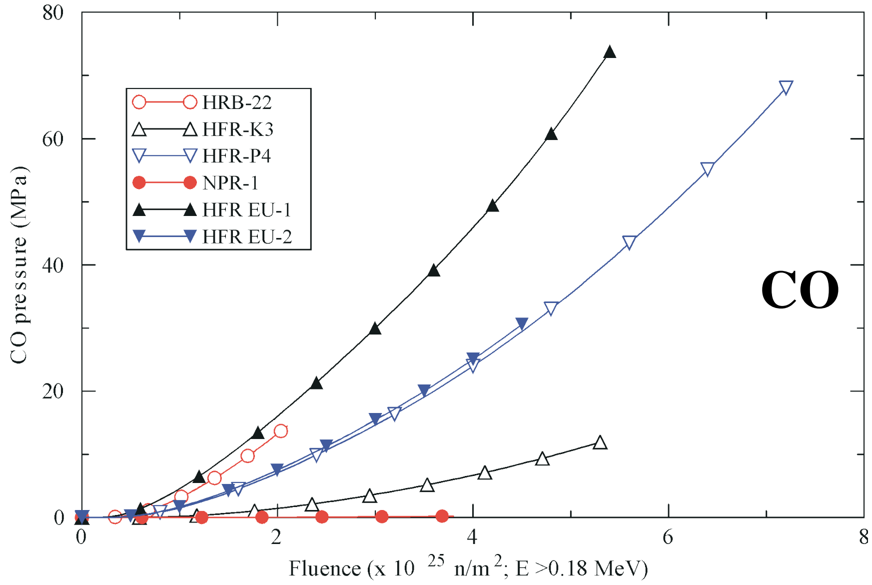


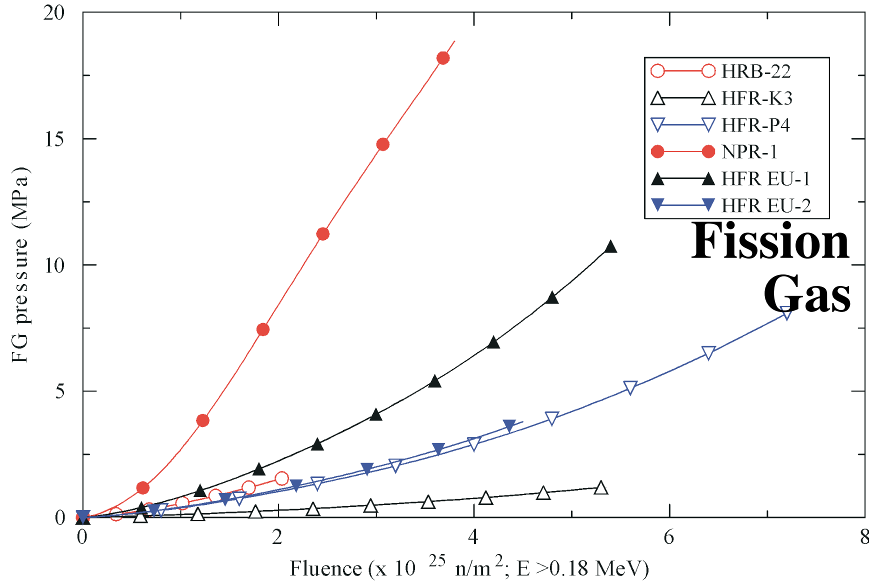
- C and Si self diffusion in β-SiC
- Cr and Fe grain boundary diffusion in β-SiC
- B and B+C grain boundary diffusion in α-SiC

Selected Applications/Benchmarks

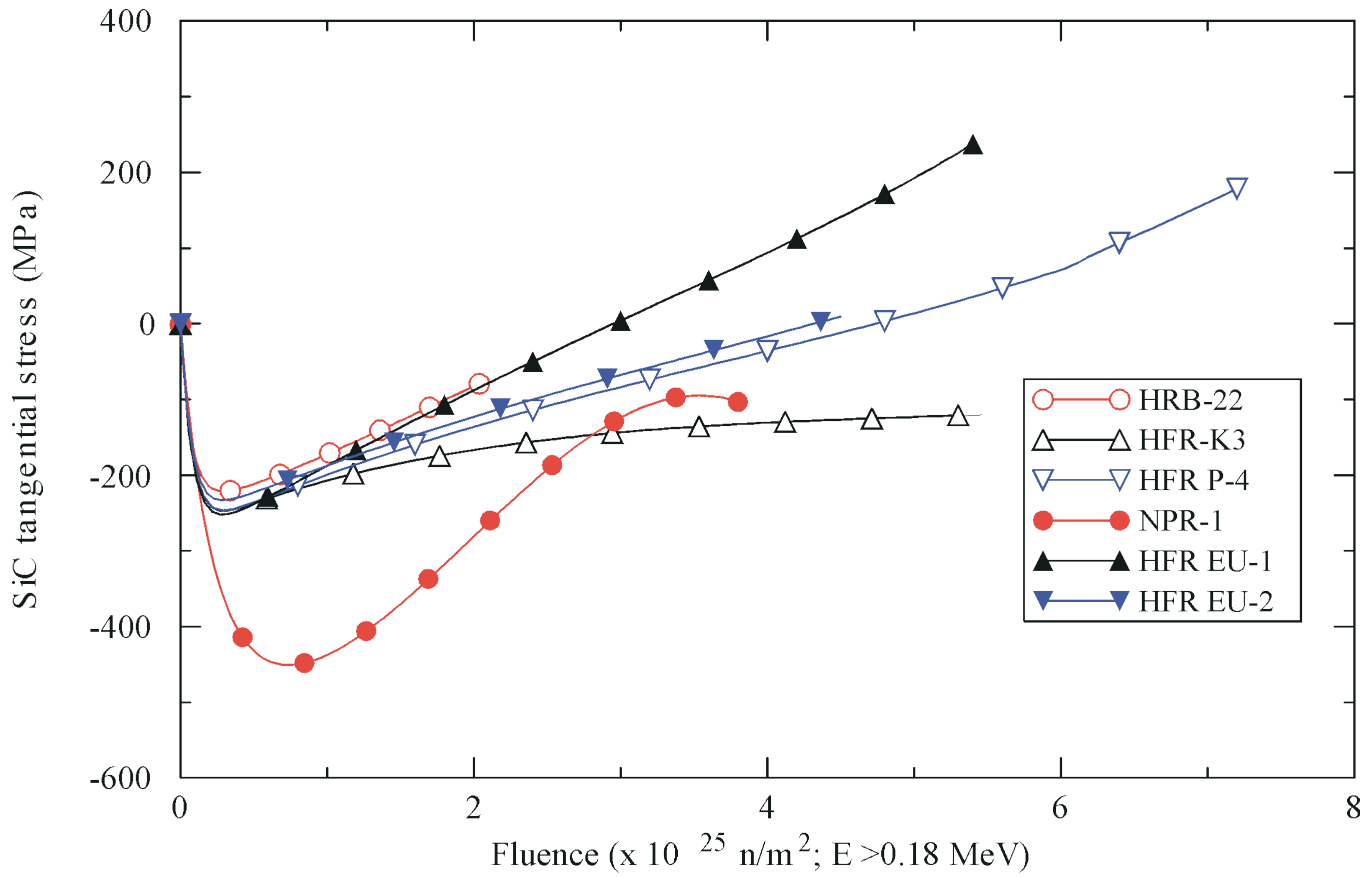
Pressures For Each Irradiation







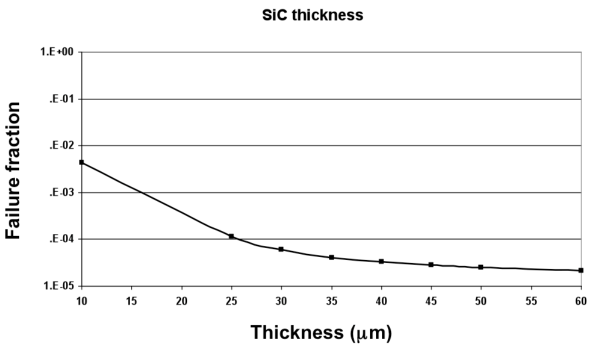
Peak SiC Stress For Each Irradiation

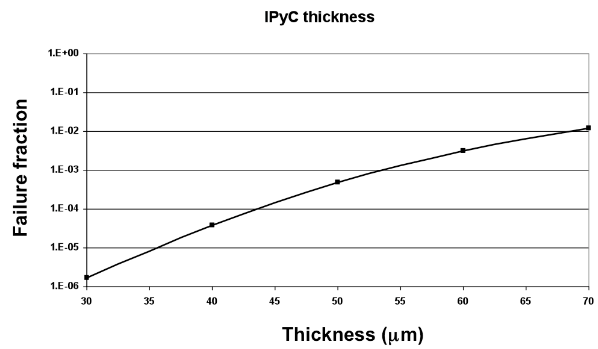


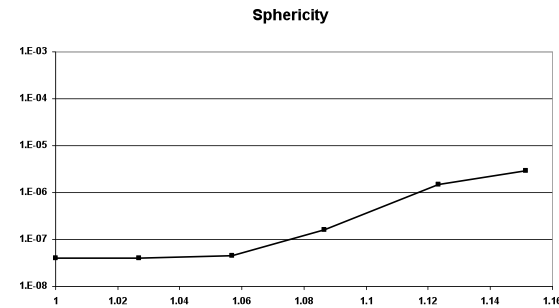
Results from Irradiation Experiments

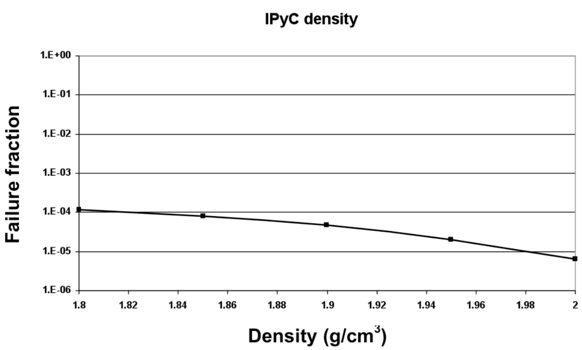
Case	Description	IPyC/SiC Bond Strength (MPa)	Probability of						
			Failure	Failure due to				IPyC Cracking	IPyC Debonding
				Amoeba	IPyC Cracking	IPyC Debonding	Pressure		
9	**HRB-22**	**100**	**4.3e-9**	**0**	**4.3e-9**	**0**	**0**	**0.17**	**0**
10	**HFR-K3**	**100**	**1.5e-7**	**0**	**1.5e-7**	**0**	**0**	**0.27**	**0**
11	**HFR-P4**	**100**	**3.6e-5**	**0**	**1.4e-7**	**0**	**3.6e-5**	**0.26**	**0**
12	**NPR-1**	**70**	**6.0e-4**	**0**	**4.6e-4**	**1.4e-4**	**0**	**0.63**	**0.36**
13	**HFR EU-1**	**100**	**7.3e-4**	**0**	**1.3e-7**	**0**	**7.3e-4**	**0.27**	**0**
14	**HFR EU-2**	**100**	**7.2e-8**	**0**	**7.2e-8**	**0**	**5.9e-10**	**0.24**	**0**

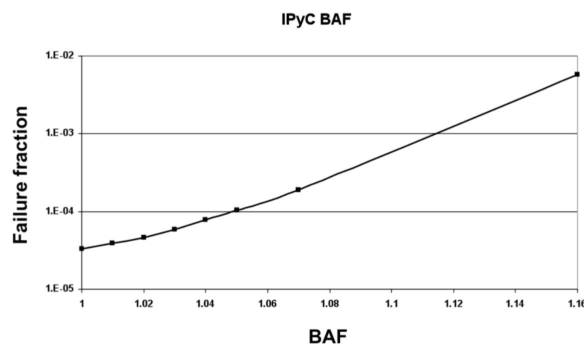
AGR-1 Sensitivity/Specification Analysis

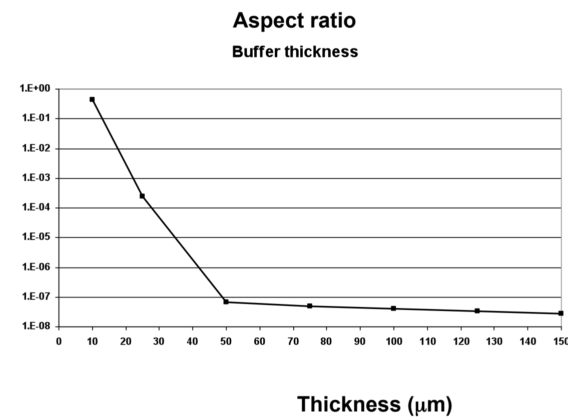




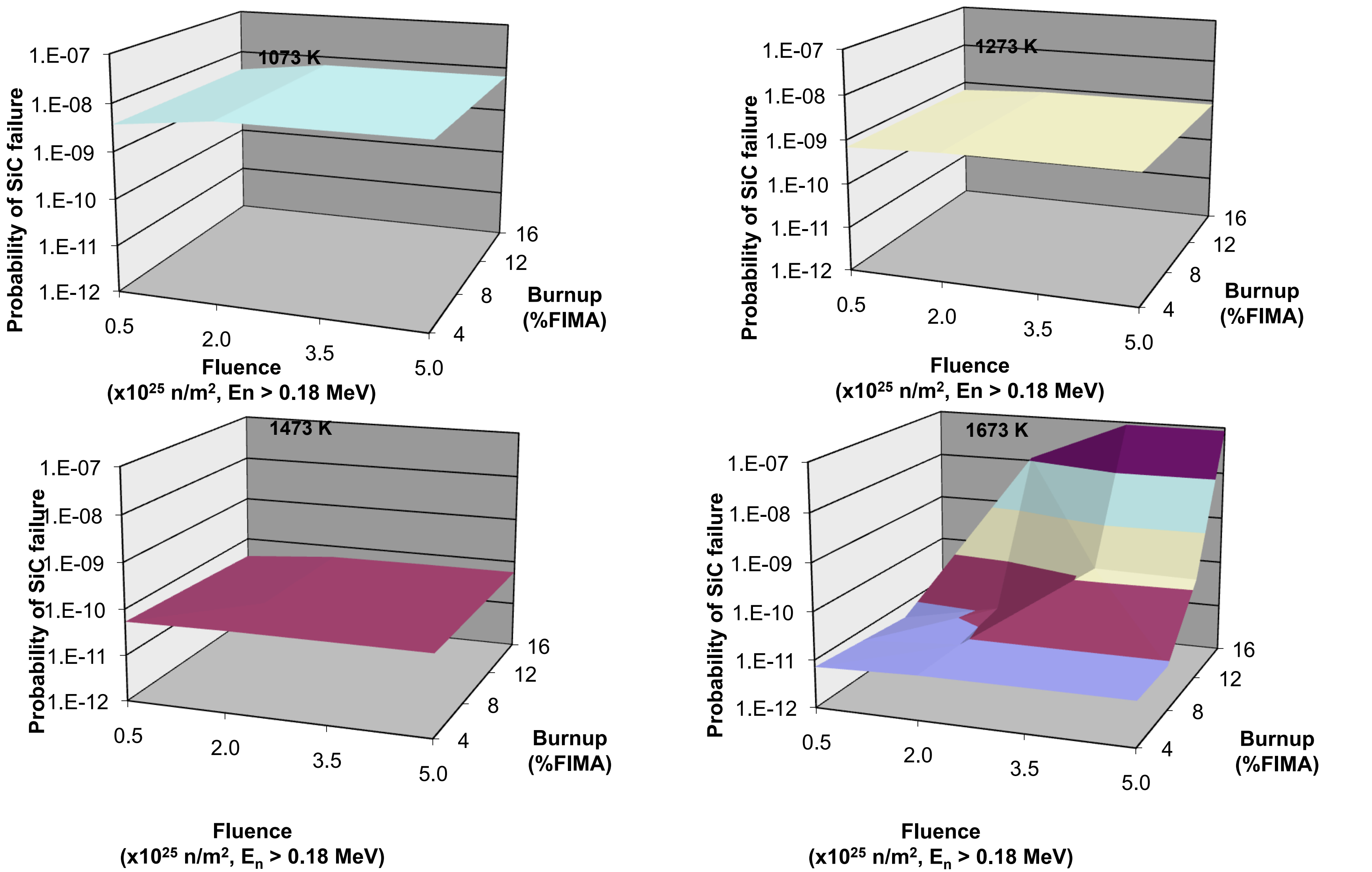








Response Surface: Evaluate effects of temperature, burnup and fluence on failure probability



Summary

- PARFUME is a mature code and the level of configuration control is being increased since it will be released outside INL in early FY-10
- PARFUME models the thermomechanical response of coated particle fuel in detail. Fission product transport models are under development and verification now.
- PARFUME predictions are limited by the current material property database. New measurements are underway or planned to improve the database
- PARFUME has undergone benchmarking as part of the IAEA normal and accident condition round robin calculations. More benchmarking is anticipated under GIF VHTR collaborations
- PARFUME has been useful in a variety of applications including evaluation of fabrication specifications, analysis of tests and predictions of reactor performance
- As the NGNP/AGR fuels program continues, there will be opportunities to test many of the models, especially under accident conditions
- Much of the physics underlying PARFUME has been captured in a soon to be released HTR Factbook to be issued by IAEA in late 2009/early 2010